

## INVENTOR SEARCH

=&gt; fil hcapl; d que nos 196

FILE 'HCAPLUS' ENTERED AT 15:37:52 ON 30 JAN 2008

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FILE COVERS 1907 - 30 Jan 2008 VOL 148 ISS 5

FILE LAST UPDATED: 29 Jan 2008 (20080129/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

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L5          1 SEA FILE=HCAPLUS ABB=ON  US2004-799286/APPS
L6          63 SEA FILE=HCAPLUS ABB=ON  BAKTHAVATCHALAM R?/AU
L7          235 SEA FILE=HCAPLUS ABB=ON  HUTCHISON A?/AU
L8          103 SEA FILE=HCAPLUS ABB=ON  DESIMONE R?/AU
L9          55 SEA FILE=HCAPLUS ABB=ON  HODGETTS K?/AU
L10         1056 SEA FILE=HCAPLUS ABB=ON  KRAUSE J?/AU
L11         2037 SEA FILE=HCAPLUS ABB=ON  WHITE G?/AU
L42         SCR 1839 AND 1993
L50         STR
L52         SCR 392 OR 391
L73         SCR 1952
L81         57965 SEA FILE=REGISTRY SSS FUL (L50) AND L42 AND L52 AND L73
L84         53736 SEA FILE=REGISTRY SSS FUL (L50) AND L42 AND L52 NOT L73
L85         111701 SEA FILE=REGISTRY ABB=ON (L81 OR L84)
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L93         8317 SEA FILE=REGISTRY SUB=L85 SSS FUL (L50 NOT (L87 OR L88 OR L89
OR L90))
L94         1407 SEA FILE=HCAPLUS ABB=ON  L93
L95         1 SEA FILE=HCAPLUS ABB=ON  L94 AND (L5 OR L6 OR L7 OR L8 OR L9
OR L10 OR L11)
L96         2 SEA FILE=HCAPLUS ABB=ON  (L95 OR L5)

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=&gt; d ibib abs hitstr 196 1-2

L96 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2002:90039 HCAPLUS Full-text  
 DOCUMENT NUMBER: 136:134792

cycloalkyl, heterocycloalkyl, or heteroaryl; n = 0, 1, and 2]. These compds. are selective modulators, in particular antagonists, of capsaicin receptors, including human capsaicin receptors, and are, therefore, useful in the treatment of a chronic and acute pain conditions, itch and urinary incontinence. The above pain is associated with a condition selected from the group consisting of postmastectomy pain syndrome, stump pain, phantom limb pain, oral neuropathic pain, Charcot's pain, toothache, venomous snake bite, spider bite, insect sting, postherpetic neuralgia, diabetic neuropathy, reflex sympathetic dystrophy, trigeminal neuralgia, osteoarthritis, rheumatoid arthritis, fibromyalgia, Guillain-Barre syndrome, meralgia paresthetica, burning-mouth syndrome, bilateral peripheral neuropathy, causalgia, sciatic neuritis, peripheral neuritis, polyneuritis, optic neuritis, postfebrile neuritis, migrating neuritis, segmental neuritis, Gombault's neuritis, neuronitis, cervicobrachial neuralgia, cranial neuralgia, geniculate neuralgia, glossopharyngeal neuralgia, migrainous neuralgia, idiopathic neuralgia, intercostals neuralgia, mammary neuralgia, mandibular joint neuralgia, Morton's neuralgia, nasociliary neuralgia, occipital neuralgia, red neuralgia, Sluder's neuralgia, splenopalatine neuralgia, supraorbital neuralgia, vidian neuralgia, sinus headache, tension headache, labor, childbirth, intestinal gas, menstruation, cancer, and trauma. Methods of treatment of such disorders as well as packaged pharmaceutical compns. are also provided. Compds. of the invention are also useful as probes for the localization of capsaicin receptors and as stds. in assays for capsaicin receptor binding and capsaicin receptor mediated cation conductance. Thus, 202 mg Et3N was added to a mixture of 212 mg (R)-1-(3-Chloropyridin-2-yl)-3-methylpiperazine and 269 mg (4-sec-Butylphenyl)carbamic acid Ph ester in CHCl3 and refluxed for 4 h to give (R)-4-(3-Chloropyridin-2-yl)-2-methylpiperazine-1-carboxylic acid (4-sec-butylphenyl)amide. Compds. I. e.g. N-(4-tert-butylphenyl)-4-(3-chloropyridin-2-yl)piperazine-1-carboxamide, in vitro showed EC50 of <1 µM in an antagonist assay for capsaicin receptor-mediated calcium mobilization using human embryonic kidney (HEK293) cells transfected with a pcDNA3.1 encoding the full length human capsaicin receptor. Methods of using the compds. in receptor localization studies are given.

L96 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:247338 HCAPLUS Full-text

DOCUMENT NUMBER: 134:280854

TITLE: Preparation of certain alkylene diamine-substituted heterocycles as NPY1 receptor inhibitors.

INVENTOR(S): Horvath, Raymond F.; Tran, Jennifer; De, Lombaert Stephane; Hodgetts, Kevin Julian; Carpino, Philip A.; Griffith, David A.

PATENT ASSIGNEE(S): Neurogen Corporation, USA; Pfizer; Inc.; De Lombaert, Stephane

SOURCE: PCT Int. Appl., 211 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

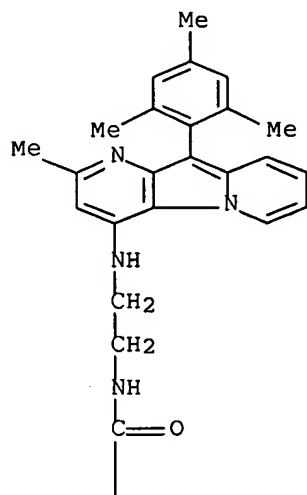
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

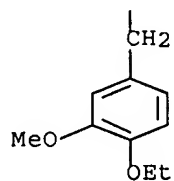
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2001023389	A2	20010405	WO 2000-US26886	20000929
WO 2001023389	A3	20020510		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,			

PAGE 1-A

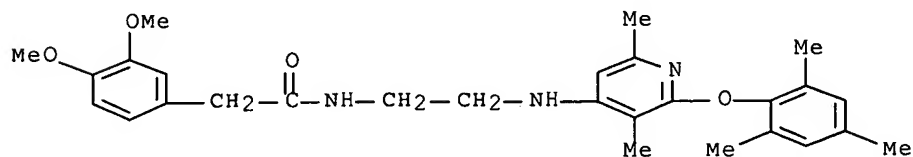


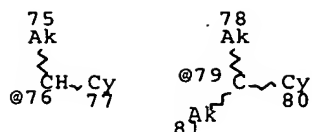
PAGE 2-A



RN 332140-80-4 HCAPLUS

CN Benzeneacetamide, N-[2-[[3,6-dimethyl-2-(2,4,6-trimethylphenoxy)-4-pyridinyl]amino]ethyl]-3,4-dimethoxy- (CA INDEX NAME)





Page 2-A

VAR G1=H/22

VAR G3=O/S

VAR G5=CY/8/11/14/16/20/21/32/34/38/43/46/50/55/60/64/69/14/76/79

NODE ATTRIBUTES:

NSPEC IS RC AT 4

NSPEC IS RC AT 5

CONNECT IS E1 RC AT 22

CONNECT IS E1 RC AT 53

CONNECT IS E1 RC AT 58

CONNECT IS E1 RC AT 59

CONNECT IS E1 RC AT 68

CONNECT IS E1 RC AT 73

CONNECT IS E1 RC AT 74

CONNECT IS E1 RC AT 75

CONNECT IS E1 RC AT 78

CONNECT IS E1 RC AT 81

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 76

STEREO ATTRIBUTES: NONE

L52 SCR 392 OR 391

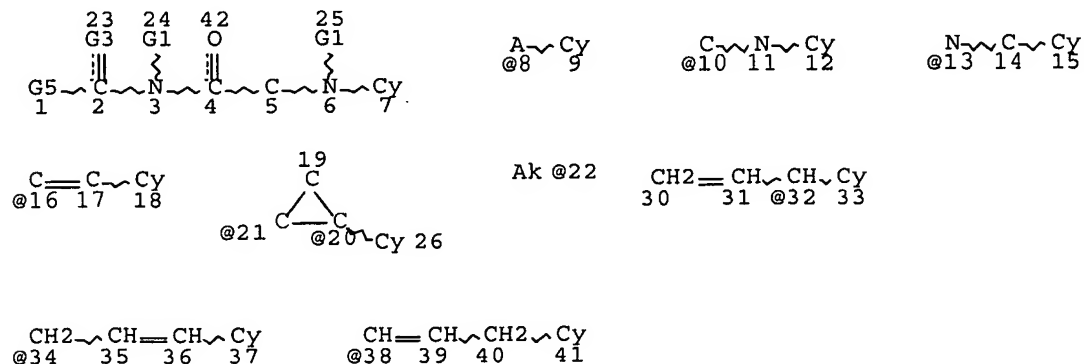
L73 SCR 1952

L81 57965 SEA FILE=REGISTRY SSS FUL (L50) AND L42 AND L52 AND L73

L84 53736 SEA FILE=REGISTRY SSS FUL (L50) AND L42 AND L52 NOT L73

L85 111701 SEA FILE=REGISTRY ABB=ON (L81 OR L84)

L87 STR STRUCTURES L87-L90 'NOT'-ed OUT OF ANSWER SET



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VAR G3=O/S

VAR G5=CY/8/10/13/16/21/20/32/34/38

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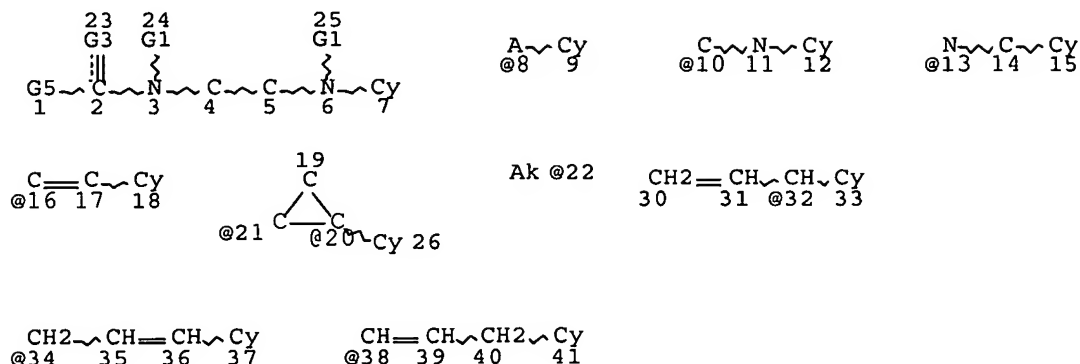
CONNECT IS E1 RC AT 22



NSPEC IS R AT 5  
 CONNECT IS E1 RC AT 22  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
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 NUMBER OF NODES IS 38

STEREO ATTRIBUTES: NONE  
 L90 STR



VAR G1=H/22  
 VAR G3=O/S  
 VAR G5=CY/8/10/13/16/21/20/32/34/38  
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 CONNECT IS E1 RC AT 22  
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 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 38

STEREO ATTRIBUTES: NONE  
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100.0% PROCESSED 111701 ITERATIONS  
 SEARCH TIME: 00.00.13

8317 ANSWERS

=> fil hcapl; d que nos 198; d que nos 1134; d que nos 1132; d que nos 1137  
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L73 SCR 1952  
 L81 57965 SEA FILE=REGISTRY SSS FUL (L50) AND L42 AND L52 AND L73  
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 L130 912 SEA FILE=HCAPLUS ABB=ON L94 AND (PY<2001 OR AY<2001 OR  
 PRY<2001)  
 L134 2 SEA FILE=HCAPLUS ABB=ON L121 AND L130  
  
 L12 13783 SEA FILE=HCAPLUS ABB=ON NEUROPATH?/OBI  
 L18 25102 SEA FILE=HCAPLUS ABB=ON PAIN/CT  
 L22 39283 SEA FILE=HCAPLUS ABB=ON ARTHRITIS/OBI  
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 L42 SCR 1839 AND 1993  
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 L52 SCR 392 OR 391  
 L73 SCR 1952  
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 PAC=PHARMACOLOGIC ACTIVITY; PKT=PHARMACOKINETICS; DMA=DRUG MECHANISM OF ACTION  
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 L14 1695 SEA FILE=HCAPLUS ABB=ON NEURALGI?/OBI  
 L15 146 SEA FILE=HCAPLUS ABB=ON CAUSALGI?/OBI  
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 L20 1574 SEA FILE=HCAPLUS ABB=ON BITE#/OBI OR STING#/OBI  
 L21 214 SEA FILE=HCAPLUS ABB=ON SYMPATHETIC/OBI(L)DYSTROPH?/OBI

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 1-((R)-5-Tert-Butyl-indan-1-yl)-3-isoquinolin-5-yl-urea (A-778317) is a novel, stereoselective, competitive antagonist that potently blocks transient receptor potential vanilloid-1 (TRPV1) receptor-mediated changes in intracellular calcium concns. ( $pIC_{50} = 8.31 \pm 0.13$ ). The (S)-stereoisomer, 1-((S)-5-tert-butyl-indan-1-yl)-3-isoquinolin-5-yl-urea (A-778316), is 6.8-fold less potent ( $pIC_{50} = 7.47 \pm 0.07$ ). A-778317 also potently blocks capsaicin and acid activation of native rat TRPV1 receptors in dorsal root ganglion neurons. A-778317 was tritiated ( $[^3H]A-778317$ ; 29.3 Ci/mmol) and used to study recombinant human TRPV1 (hTRPV1) receptors expressed in Chinese ovary cells (CHO) cells.  $[^3H]A-778317$  labeled a single class of binding sites in hTRPV1-expressing CHO cell membranes with high affinity ( $K_D = 3.4$  nM;  $B_{max} = 4.0$  pmol/mg protein). Specific binding of 2 nM  $[^3H]A-778317$  to hTRPV1-expressing CHO cell membranes was reversible. The rank-order potency of TRPV1 receptor antagonists to inhibit binding of 2 nM  $[^3H]A-778317$  correlated well with their functional potencies in blocking TRPV1 receptor activation. The present data demonstrate that A-778317 blocks polymodal activation of the TRPV1 receptor by binding to a single high-affinity binding site and that  $[^3H]A-778317$  possesses favorable binding properties to facilitate further studies of hTRPV1 receptor pharmacol.

CC 1-1 (Pharmacology)

Section cross-reference(s): 2

IT Capsaicin receptors

RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 (type VR1;  $[^3H]A-778317$  [1-((R)-5-tert-Bu-indan-1-yl)-3-isoquinolin-5-yl-urea], a novel, stereoselective, high-affinity antagonist is a useful radioligand for human transient receptor potential vanilloid-1 (TRPV1) receptor)

IT 7440-70-2, Calcium, biological studies 459429-39-1, SB-452533  
 545398-74-1, AMG6880 581809-67-8, A-425619 628719-73-3 808756-63-0,  
 A 778316 808756-64-1, A 778317 824982-41-4, A-784168

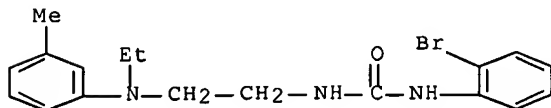
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 ( $[^3H]A-778317$  [1-((R)-5-tert-Bu-indan-1-yl)-3-isoquinolin-5-yl-urea], a novel, stereoselective, high-affinity antagonist is a useful radioligand for human transient receptor potential vanilloid-1 (TRPV1) receptor)

IT 459429-39-1, SB-452533

RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 ( $[^3H]A-778317$  [1-((R)-5-tert-Bu-indan-1-yl)-3-isoquinolin-5-yl-urea], a novel, stereoselective, high-affinity antagonist is a useful radioligand for human transient receptor potential vanilloid-1 (TRPV1) receptor)

RN 459429-39-1 HCAPLUS

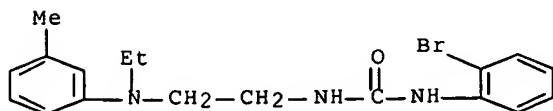
CN Urea, N-(2-bromophenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]- (CA  
 INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 2 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2007:653928 HCAPLUS Full-text

IT 459429-39-1D, SB-452533, derivative  
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL  
 (Biological study); USES (Uses)  
 (characterization of SB-705498, a potent and selective vanilloid  
 receptor-1 (VR1/TRPV1) antagonist that inhibits the capsaicin-, acid-,  
 and heat-mediated activation of receptor)  
 RN 459429-39-1 HCAPLUS  
 CN Urea, N-(2-bromophenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]- (CA  
 INDEX NAME)



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 3 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:175521 HCAPLUS Full-text

DOCUMENT NUMBER: 146:229352

TITLE: Substituted benzimidazole compounds as dual nitric  
 oxide synthase inhibitors and  $\mu$ -opioid agonists,  
 their preparation, pharmaceutical compositions, and  
 use in therapy

INVENTOR(S): Renton, Paul; Maddaford, Shawn; Rakhit, Suman;  
 Andrews, John

PATENT ASSIGNEE(S): Neuraxon, Inc., Can.

SOURCE: PCT Int. Appl., 139pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007017764	A2	20070215	WO 2006-IB3075	20060518
WO 2007017764	A3	20070705		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
AU 2006277684	A1	20070215	AU 2006-277684	20060518
PRIORITY APPLN. INFO.:			US 2005-682043P	P 20050518
			WO 2006-IB3075	W 20060518

OTHER SOURCE(S): MARPAT 146:229352

GI

N-(2-Amino-5-nitrophenyl)-2-(4-ethoxyphenyl)acetamide 925216-76-8P,  
 (2,4-Dinitrophenyl)(1-methylpiperidin-4-yl)amine 925216-77-9P,  
 1-[(1-Methylpiperidin-4-yl)amino]-4-nitrobenzene-2-amine  
 925216-78-0P, 2-(4-Ethoxyphenyl)-N-[2-(1-methylpiperidin-4-ylamino)-5-nitrophenyl]acetamide 925216-79-1P, 2-(4-Ethoxybenzyl)-1-(1-methylpiperidin-4-yl)-5-nitro-1H-benzimidazole 925216-81-5P,  
 1-(1-Methylpiperidin-4-yl)-5-nitro-1H-benzimidazole  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of benzimidazole compds. as dual nitric oxide synthase inhibitors and  $\mu$ -opioid agonists)

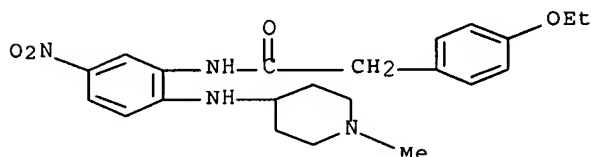
IT 925216-78-0P, 2-(4-Ethoxyphenyl)-N-[2-(1-methylpiperidin-4-ylamino)-5-nitrophenyl]acetamide

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of benzimidazole compds. as dual nitric oxide synthase inhibitors and  $\mu$ -opioid agonists)

RN 925216-78-0 HCAPLUS

CN Benzeneacetamide, 4-ethoxy-N-[2-[(1-methyl-4-piperidiny]amino)-5-nitrophenyl]- (CA INDEX NAME)



L163 ANSWER 4 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:453918 HCAPLUS Full-text

DOCUMENT NUMBER: 145:76019

TITLE: Discovery of SB-705498: A potent, selective and orally bioavailable TRPV1 antagonist suitable for clinical development

AUTHOR(S): Rami, Harshad K.; Thompson, Mervyn; Stemp, Geoffrey; Fell, Steve; Jerman, Jeffrey C.; Stevens, Alexander J.; Smart, Darren; Sargent, Becky; Sanderson, Dominic; Randall, Andrew D.; Gunthorpe, Martin J.; Davis, John B.

CORPORATE SOURCE: Neurology and GI CEDD, GlaxoSmithKline, Essex, CM19 5AW, UK

SOURCE: Bioorganic & Medicinal Chemistry Letters (2006), 16(12), 3287-3291

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

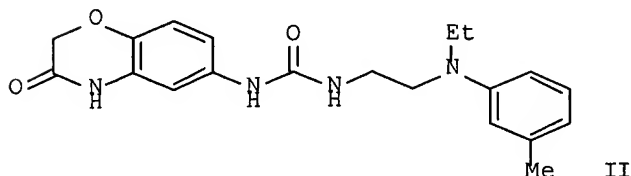
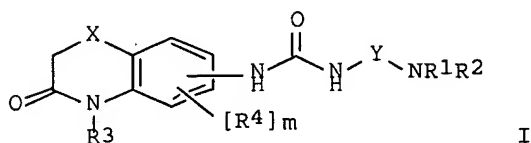
OTHER SOURCE(S): CASREACT 145:76019

GI

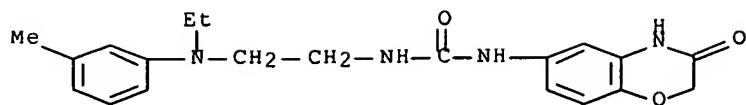
vanilloid receptor antagonists  
 INVENTOR(S): Fujishima, Hiroshi; Mogi, Muneto; Yuasa, Hiroaki;  
 Taijimi, Masaomi; Yamamoto, Noriyuki; Hayashi,  
 Fumihiko; Tsukimi, Yasuhiro; Gupta, Jang  
 PATENT ASSIGNEE(S): Bayer Healthcare AG, Germany  
 SOURCE: PCT Int. Appl., 53 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005103018	A1	20051103	WO 2005-EP3632	20050407
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2563494	A1	20051103	CA 2005-2563494	20050407
EP 1740557	A1	20070110	EP 2005-716548	20050407
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
JP 2007533673	T	20071122	JP 2007-508757	20050407
PRIORITY APPLN. INFO.:			EP 2004-9274	A 20040420
			WO 2005-EP3632	W 20050407
OTHER SOURCE(S):			CASREACT 143:440424; MARPAT 143:440424	

GI

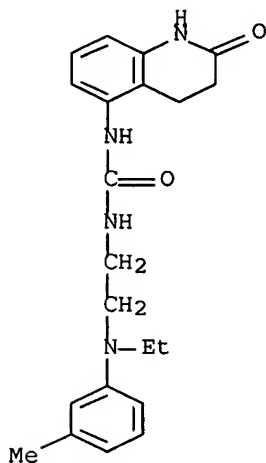


AB The invention is related to ureas (I), tautomers, stereoisomers, and salts thereof [wherein Y = (CH<sub>2</sub>)<sub>n</sub>; n = 0-4; R<sub>1</sub> = (un)substituted 3-8 membered (un)saturated ring; R<sub>2</sub> = H, (un)substituted alk(en/yn)yl, cycloalkyl, etc.;



RN 868593-16-2 HCAPLUS

CN Urea, N-[2-[ethyl(3-methylphenyl)amino]ethyl]-N'-(1,2,3,4-tetrahydro-2-oxo-5-quinoliny)- (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 6 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:429388 HCAPLUS Full-text

DOCUMENT NUMBER: 142:463465

TITLE: Preparation of bicyclic amide, carbamate or urea derivatives as vanilloid receptor modulators

INVENTOR(S): Mogi, Muneto; Fujishima, Hiroshi; Tajimi, Masaomi; Yamamoto, Noriyuki; Urbahns, Klaus; Hayashi, Fumihiko; Tsukimi, Yasuhiro; Gupta, Jang; Yuasa, Hiroaki

PATENT ASSIGNEE(S): Bayer Healthcare A.-G., Germany

SOURCE: PCT Int. Appl., 63 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005044786	A1	20050519	WO 2004-EP12050	20041026
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,				

vanilloid receptor antagonists)

IT 851773-81-4P, N-[4-Chloro-3-(trifluoromethyl)phenyl]-N'-(7-hydroxy-5,6,7,8-tetrahydronaphthalen-2-yl)urea 851773-82-5P, N-(7-Hydroxy-5,6,7,8-tetrahydronaphthalen-2-yl)-N'-[4-(trifluoromethyl)benzyl]urea 851773-83-6P, 4-(Trifluoromethyl)benzyl (7-hydroxy-5,6,7,8-tetrahydronaphthalen-2-yl)carbamate 851773-84-7P, N-(7-Hydroxy-5,6,7,8-tetrahydronaphthalen-2-yl)-3-[4-(trifluoromethyl)phenyl]propanamide 851773-85-8P, N-(7-Hydroxy-5,6,7,8-tetrahydronaphthalen-2-yl)-N'-[2-[[4-(trifluoromethyl)phenyl]amino]ethyl]urea 851773-86-9P, N-(7-Hydroxy-5,6,7,8-tetrahydronaphthalen-2-yl)-N'-[2-[4-(trifluoromethyl)phenoxy]ethyl]urea 851773-87-0P, 2-[[4-(Trifluoromethyl)phenyl]amino]ethyl (7-hydroxy-5,6,7,8-tetrahydronaphthalen-2-yl)carbamate 851773-88-1P, 2-[4-(Trifluoromethyl)phenoxy]ethyl (7-hydroxy-5,6,7,8-tetrahydronaphthalen-2-yl)carbamate 851773-89-2P, N-[2-[[4-Chloro-3-(trifluoromethyl)phenyl]amino]ethyl]-N'-(7-hydroxy-5,6,7,8-tetrahydronaphthalen-2-yl)urea 851773-90-5P, N-[2-[4-Chloro-3-(trifluoromethyl)phenoxy]ethyl]-N'-(7-hydroxy-5,6,7,8-tetrahydronaphthalen-2-yl)urea 851773-91-6P, N-[2-[[4-Chloro-3-(trifluoromethyl)phenyl]amino]ethyl]-N'-(6-hydroxy-5,6,7,8-tetrahydronaphthalen-2-yl)urea 851773-92-7P, N-[2-[4-Chloro-3-(trifluoromethyl)phenoxy]ethyl]-N'-(6-hydroxy-5,6,7,8-tetrahydronaphthalen-2-yl)urea  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

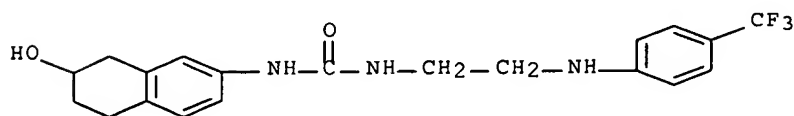
(preparation of bicyclic amides, carbamates or urea derivs. as vanilloid receptor antagonists)

IT 851773-85-8P, N-(7-Hydroxy-5,6,7,8-tetrahydronaphthalen-2-yl)-N'-[2-[[4-(trifluoromethyl)phenyl]amino]ethyl]urea 851773-89-2P, N-[2-[[4-Chloro-3-(trifluoromethyl)phenyl]amino]ethyl]-N'-(7-hydroxy-5,6,7,8-tetrahydronaphthalen-2-yl)urea 851773-91-6P, N-[2-[[4-Chloro-3-(trifluoromethyl)phenyl]amino]ethyl]-N'-(6-hydroxy-5,6,7,8-tetrahydronaphthalen-2-yl)urea  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of bicyclic amides, carbamates or urea derivs. as vanilloid receptor antagonists)

RN 851773-85-8 HCAPLUS

CN Urea, N-(5,6,7,8-tetrahydro-7-hydroxy-2-naphthalenyl)-N'-[2-[[4-(trifluoromethyl)phenyl]amino]ethyl]- (CA INDEX NAME)

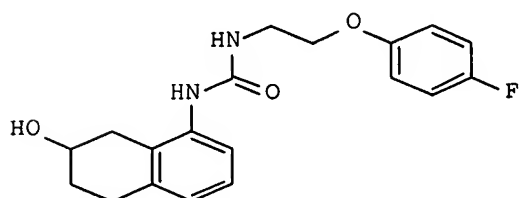
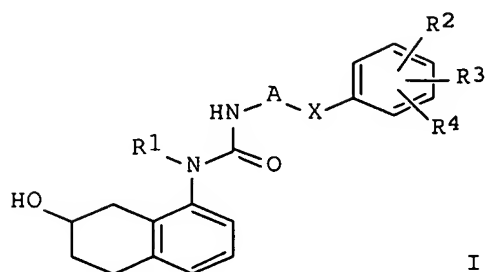


RN 851773-89-2 HCAPLUS

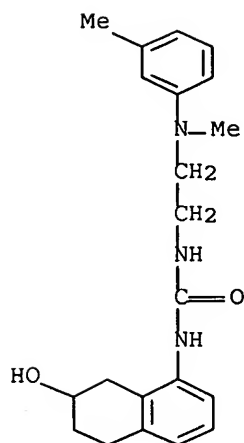
CN Urea, N-[2-[[4-chloro-3-(trifluoromethyl)phenyl]amino]ethyl]-N'-(5,6,7,8-tetrahydro-7-hydroxy-2-naphthalenyl)- (CA INDEX NAME)



IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK  
 JP 2006517556 T 20060727 JP 2006-501742 20040205  
 US 2007027187 A1 20070201 US 2004-545556 20040205  
 PRIORITY APPLN. INFO.: EP 2003-2672 A 20030212  
 WO 2004-EP1055 W 20040205  
 OTHER SOURCE(S): MARPAT 141:225165  
 GI



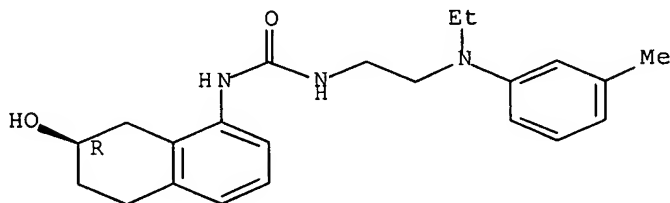
- AB This invention relates to hydroxytetrahydronaphthalenylurea derivs. of formula I, wherein A = (CH<sub>2</sub>)<sub>n</sub>; n is 1-6; R<sub>1</sub> is H or alkyl; R<sub>2</sub>, R<sub>3</sub> and R<sub>4</sub> are independently H, halo, hydroxy, (di)alkylamino, cycloalkylamino, alkoxy carbonyl, Ph, benzyl, sulfonamide, alkanoyl(amino), (alkyl)carbamoyl, cyano(alkyl), (un)substituted alkoxy, phenoxy, or alkylthio; X is O, S, NR<sub>5</sub>; R<sub>5</sub> is H, benzyl or alkyl, and tautomeric or stereoisomers and physiolog. acceptable salts thereof, which are useful as active ingredients of pharmaceutical preps. The compds. have been synthesized as VR1 antagonists, and can be used for the prophylaxis and treatment of diseases associated with VR1 activity, in particular for the treatment of urol. disorders or diseases, pain and inflammatory disorders or diseases. Thus, urea II and its enantiomers were prepared in several steps from 8-amino-2-naphthol and 2-(4-fluorophenoxy)ethylamine. The effects of the compds. were examined in the following several assays and pharmacol. tests: measurement of capsaicin-induced Ca<sup>2+</sup> influx in a human VR1-transfected CHO cell line and in primary cultured rat dorsal root ganglia neurons, resp., measurement of capsaicin-induced bladder contraction, measurement of overactive bladder in anesthetized cystitis rats, measurement of acute pain, persistent pain, neuropathic pain, inflammatory pain and diabetic neuropathic pain (only the 1st assay had data). II and its two enantiomers all showed ≤ 0.1 μM of IC<sub>50</sub> in the 1st assay. Specifically disclosed applications of I include the treatment of urinary incontinence, urge urinary incontinence, overactive bladder, chronic pain, neuropathic pain, postoperative pain, rheumatoid arthritic pain, neuralgia, neuropathies, algesia, nerve injury, ischemia, neurodegeneration, stroke, inflammatory disorders, asthma and COPD.
- IC ICM C07C275-32  
 ICS C07D295-08; A61K031-17; A61K031-44; A61P013-00; A61P025-00



RN 745784-24-1 HCAPLUS

CN Urea, N-[2-[ethyl(3-methylphenyl)amino]ethyl]-N'-[(7R)-5,6,7,8-tetrahydro-7-hydroxy-1-naphthalenyl]- (CA INDEX NAME)

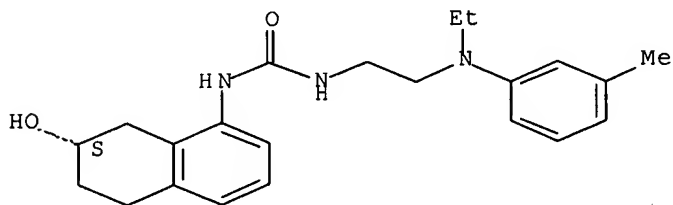
Absolute stereochemistry.



RN 745784-25-2 HCAPLUS

CN Urea, N-[2-[ethyl(3-methylphenyl)amino]ethyl]-N'-[(7S)-5,6,7,8-tetrahydro-7-hydroxy-1-naphthalenyl]- (CA INDEX NAME)

Absolute stereochemistry.



L163 ANSWER 8 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:498554 HCAPLUS [Full-text](#)

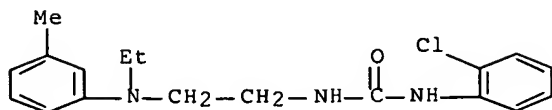
DOCUMENT NUMBER: 141:133552

TITLE: Discovery of small molecule antagonists of TRPV1

AUTHOR(S): Rami, Harshad K.; Thompson, Mervyn; Wyman, Paul; Jerman, Jeffrey C.; Egerton, Julie; Brough, Stephen; Stevens, Alexander J.; Randall, Andrew D.; Smart, Darren; Gunthorpe, Martin J.; Davis, John B.

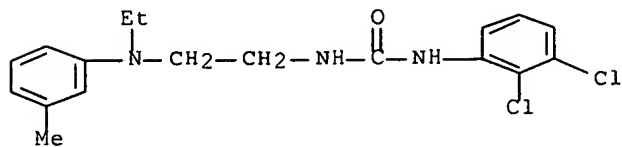
RN 459429-44-8 HCAPLUS

CN Urea, N-(2-chlorophenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl] - (CA INDEX NAME)



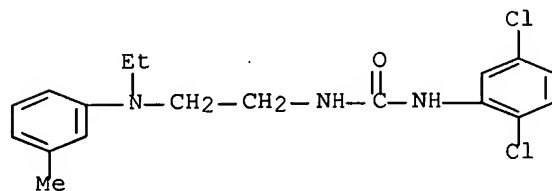
RN 459429-55-1 HCAPLUS

CN Urea, N-(2,3-dichlorophenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl] - (CA INDEX NAME)



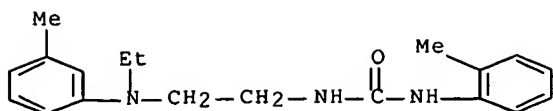
RN 459429-56-2 HCAPLUS

CN Urea, N-(2,5-dichlorophenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl] - (CA INDEX NAME)



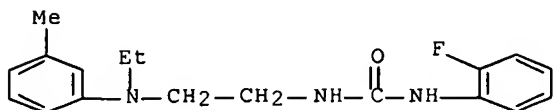
RN 459429-59-5 HCAPLUS

CN Urea, N-[2-[ethyl(3-methylphenyl)amino]ethyl]-N'-1-naphthalenyl - (CA INDEX NAME)



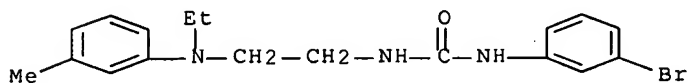
RN 725746-49-6 HCAPLUS

CN Urea, N-[2-[ethyl(3-methylphenyl)amino]ethyl]-N'-(2-fluorophenyl)- (CA INDEX NAME)



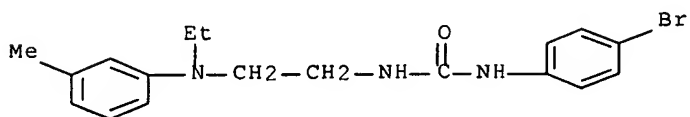
RN 725746-50-9 HCAPLUS

CN Urea, N-(3-bromophenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]- (CA INDEX NAME)



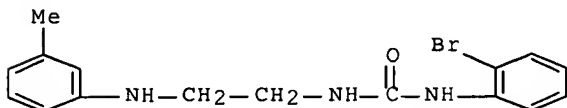
RN 725746-51-0 HCAPLUS

CN Urea, N-(4-bromophenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]- (CA INDEX NAME)



RN 725746-52-1 HCAPLUS

CN Urea, N-(2-bromophenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]- (CA INDEX NAME)



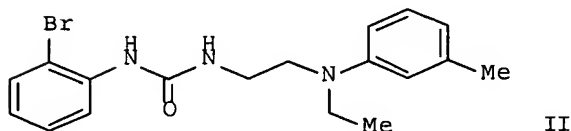
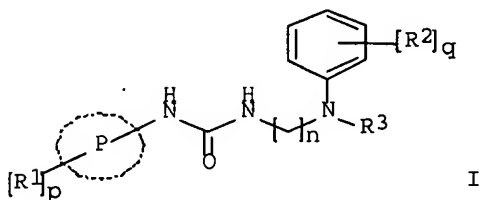
RN 725746-53-2 HCAPLUS

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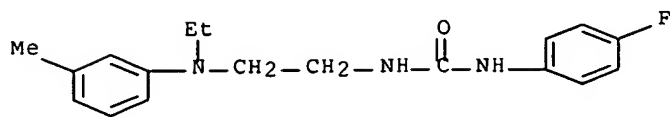
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 9 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2002:716238 HCAPLUS Full-text  
 DOCUMENT NUMBER: 137:232456  
 TITLE: Preparation of ureas having vanilloid receptor (VR1) antagonist activity  
 INVENTOR(S): Thompson, Mervyn; Wyman, Paul Adrian  
 PATENT ASSIGNEE(S): Smithkline Beecham P.L.C., UK; Glaxosmithkline  
 SOURCE: PCT Int. Appl., 18 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002072536	A1	20020919	WO 2002-GB1046	20020307
WO 2002072536	A8	20030109		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002238732	A1	20020924	AU 2002-238732	20020307
EP 1366020	A1	20031203	EP 2002-704932	20020307
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004525127	T	20040819	JP 2002-571452	20020307
US 2004082661	A1	20040429	US 2003-471393	20030908
PRIORITY APPLN. INFO.:			GB 2001-5895	A 20010309
			WO 2002-GB1046	W 20020307
OTHER SOURCE(S):		MARPAT 137:232456		
GI				

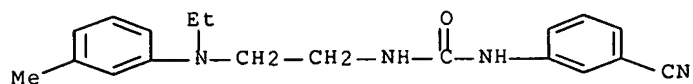


CN Urea, N-[2-[ethyl(3-methylphenyl)amino]ethyl]-N'-(4-fluorophenyl)- (CA INDEX NAME)



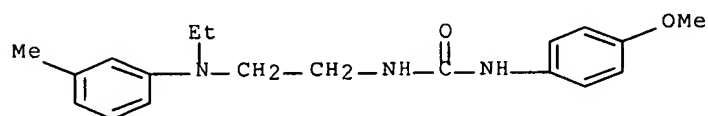
RN 459429-42-6 HCAPLUS

CN Urea, N-(3-cyanophenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]- (CA INDEX NAME)



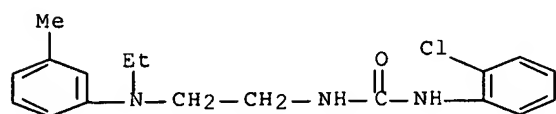
RN 459429-43-7 HCAPLUS

CN Urea, N-[2-[ethyl(3-methylphenyl)amino]ethyl]-N'-(4-methoxyphenyl)- (CA INDEX NAME)



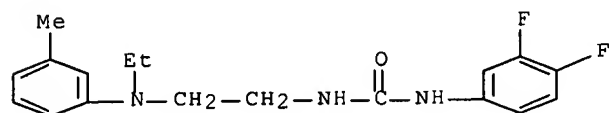
RN 459429-44-8 HCAPLUS

CN Urea, N-(2-chlorophenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]- (CA INDEX NAME)



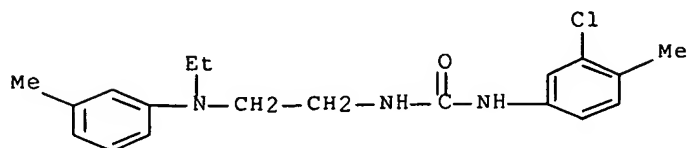
RN 459429-45-9 HCAPLUS

CN Urea, N-(3,4-difluorophenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]- (CA INDEX NAME)



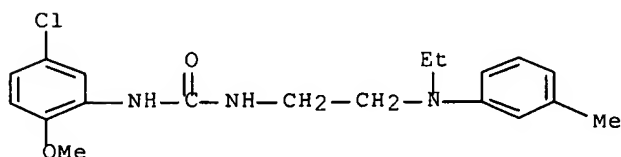
RN 459429-51-7 HCAPLUS

CN Urea, N-(3-chloro-4-methylphenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]-(CA INDEX NAME)



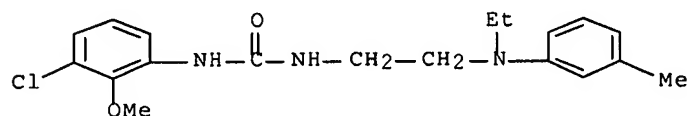
RN 459429-52-8 HCAPLUS

CN Urea, N-(5-chloro-2-methoxyphenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]-(CA INDEX NAME)



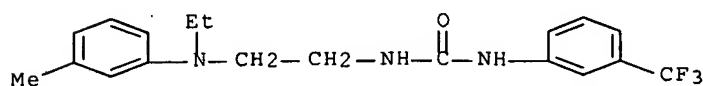
RN 459429-53-9 HCAPLUS

CN Urea, N-(3-chloro-2-methoxyphenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]-(CA INDEX NAME)



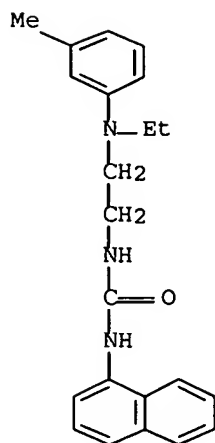
RN 459429-54-0 HCAPLUS

CN Urea, N-[2-[ethyl(3-methylphenyl)amino]ethyl]-N'-[3-(trifluoromethyl)phenyl]-(CA INDEX NAME)



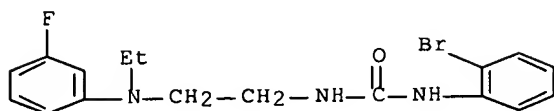
RN 459429-55-1 HCAPLUS

CN Urea, N-(2,3-dichlorophenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]-(CA INDEX NAME)



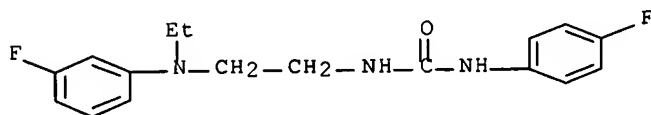
RN 459429-60-8 HCAPLUS

CN Urea, N-(2-bromophenyl)-N'-[2-[ethyl(3-fluorophenyl)amino]ethyl] - (CA INDEX NAME)



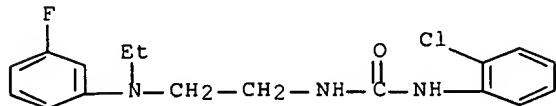
RN 459429-61-9 HCAPLUS

CN Urea, N-[2-[ethyl(3-fluorophenyl)amino]ethyl]-N'-(4-fluorophenyl) - (CA INDEX NAME)



RN 459429-62-0 HCAPLUS

CN Urea, N-(2-chlorophenyl)-N'-[2-[ethyl(3-fluorophenyl)amino]ethyl] - (CA INDEX NAME)

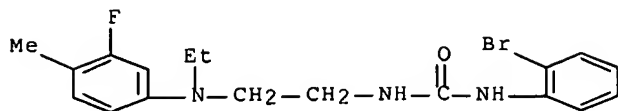


RN 459429-63-1 HCAPLUS

CN Urea, N-(3-chloro-2-methylphenyl)-N'-[2-[ethyl(3-fluorophenyl)amino]ethyl] - (CA INDEX NAME)

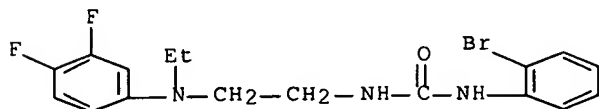


CN Urea, N-(2-bromophenyl)-N'-[2-[ethyl(3-fluoro-4-methylphenyl)amino]ethyl] -  
(CA INDEX NAME)



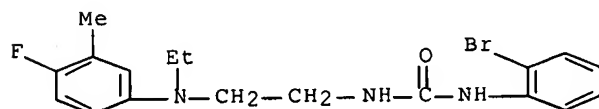
RN 459429-68-6 HCAPLUS

CN Urea, N-(2-bromophenyl)-N'-[2-[(3,4-difluorophenyl)ethylamino]ethyl] - (CA  
INDEX NAME)



RN 459429-69-7 HCAPLUS

CN Urea, N-(2-bromophenyl)-N'-[2-[ethyl(4-fluoro-3-methylphenyl)amino]ethyl] -  
(CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 10 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:575047 HCAPLUS Full-text

DOCUMENT NUMBER: 137:140533

TITLE: Preparation of 2,4,8-trisubstituted-8H-pyrido[2,3-  
d]pyrimidin-7-ones as CSBP/RK/p38 kinase inhibitors

INVENTOR(S): Adams, Jerry L.; Boehm, Jeffrey C.; Hall, Ralph; Jin,  
Qi; Kaspavec, Jiri; Silva, Domingos J.; Taggart, John  
J.

PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA

SOURCE: PCT Int. Appl., 203 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002059083	A2	20020801	WO 2001-US50493	20011023 <--
WO 2002059083	A3	20030410		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

independently H or (un)substituted alkyl, cycloalkyl(alkyl), or aryl(alkyl); or NR<sub>4</sub>R<sub>14</sub> = (un)substituted heterocyclyl; R<sub>10</sub> = H or alkyl; n = 0-10] were prepared as CSBP/p38 kinase inhibitors. For example, sequential coupling of 4,6-dichloro-2-methylsulfanylpurimidine-5- carbaldehyde with aniline (76%) and phenylboronic acid (70%) gave 2-methylsulfanyl-4-phenyl-6-phenylaminopyrimidine-5-carbaldehyde. Cyclization with bis(2,2,2-trifluoroethyl)(methoxycarbonylmethyl)phosphonate in the presence of 18-crown-6 and bis(trimethylsilyl)amide in THF afforded the 8H-pyrido[2,3-d]pyrimidin-7-one II (91%). The latter exhibited pos. inhibitory activity in the CSBP/p38 kinase binding assay with IC<sub>50</sub> < 10  $\mu$ M. I are useful for the treatment of a variety of CSBP/p38 kinase mediated diseases, such as arthritis, sepsis, stroke, asthma, pulmonary disease, osteoporosis, congestive heart failure, the common cold or respiratory viral infections, etc. (no data).

IC ICM C07D

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

IT Arthritis

(Reiter's syndrome; preparation of pyridopyrimidinones as CSBP/RK/p38

kinase

inhibitors by cyclization reactions of (phenylamino)pyrimidinecarbaldehyde derivs.)

IT Angiogenesis inhibitors

Anti-ischemic agents

Antiarthritics

Antiasthmatics

Antibacterial agents

Anticoagulants

Antidiabetic agents

Antimalarials

Antirheumatic agents

Antitumor agents

Antiviral agents

Arthritis

Asthma

Bone resorption

Bone resorption inhibitors

Cardiovascular agents

Common cold

Coronary bypass surgery

Eczema

Gout

Influenza

Malaria

Meningitis

Neoplasm

Nervous system agents

Osteoarthritis

Osteoporosis

Pneumonia

Psoriasis

Rheumatoid arthritis

Sepsis

Silicosis

Sunburn

Thrombosis

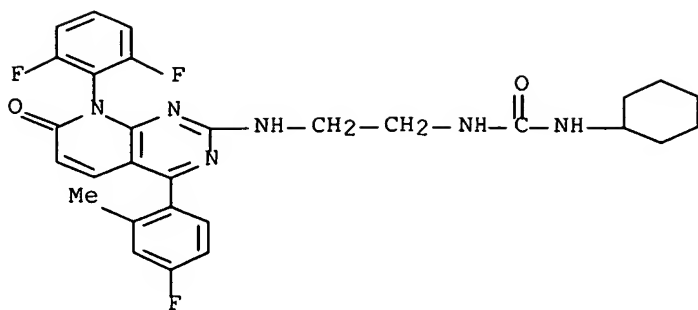
(preparation of pyridopyrimidinones as CSBP/RK/p38 kinase inhibitors by cyclization reactions of (phenylamino)pyrimidinecarbaldehyde derivs.)

IT Arthritis

Synovial membrane, disease

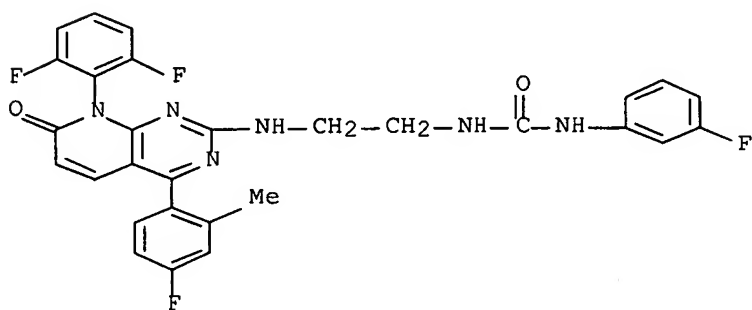
d]pyrimidin-7-one 444606-68-2P, N-(7-Oxo-4,8-diphenyl-7,8-dihydropyrido[2,3-d]pyrimidin-2-yl)methanesulfonamide 444606-69-3P, N-[4,8-Bis(2-fluorophenyl)-7-oxo-7,8-dihydropyrido[2,3-d]pyrimidin-2-yl)methanesulfonamide 444606-71-7P, N-[4-(2-Fluorophenyl)-8-isopropyl-7-oxo-7,8-dihydropyrido[2,3-d]pyrimidin-2-yl)methanesulfonamide 444606-73-9P, N-[8-(2,6-Difluorophenyl)-4-(2-fluorophenyl)-7-oxo-7,8-dihydropyrido[2,3-d]pyrimidin-2-yl)methanesulfonamide 444606-78-4P, 8-(2,6-Difluorophenyl)-2-ethoxy-4-(4-fluoro-2-methylphenyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444606-79-5P, 2-Butoxy-8-(2,6-difluorophenyl)-4-(4-fluoro-2-methylphenyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444606-81-9P, 8-(2-Chlorophenyl)-4-(2-fluorophenyl)-2-methoxy-8H-pyrido[2,3-d]pyrimidin-7-one 444606-85-3P, 8-(1-Ethylpropyl)-4-(4-fluoro-2-methylphenyl)-2-methoxy-8H-pyrido[2,3-d]pyrimidin-7-one 444606-89-7P, 4,8-Bis(2-chlorophenyl)-2-(2-hydroxyethoxy)-8H-pyrido[2,3-d]pyrimidin-7-one 444606-93-3P, 4-(2-Fluorophenyl)-8-methyl-2-methylsulfanyl-8H-pyrido[2,3-d]pyrimidin-7-one 444606-94-4P, 8-Ethyl-4-(2-fluorophenyl)-2-methylsulfanyl-8H-pyrido[2,3-d]pyrimidin-7-one 444606-98-8P, 8-(2-Chlorophenyl)-2-methylsulfanyl-4-phenoxy-8H-pyrido[2,3-d]pyrimidin-7-one 444606-99-9P, 2-Amino-8-(2,6-difluorophenyl)-4-(2-fluorophenyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-00-5P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-methylsulfanyl-5,8-dihydro-6H-pyrido[2,3-d]pyrimidin-7-one 444607-04-9P, 2-[(2-Diethylaminoethyl)amino]-8-(2,6-difluorophenyl)-4-(4-fluoro-2-methylphenyl)-5,8-dihydro-6H-pyrido[2,3-d]pyrimidin-7-one 444607-06-1P, 4-(4-Fluoro-2-methylphenyl)-2-(2-hydroxyethylamino)-8-isopropyl-8H-pyrido[2,3-d]pyrimidin-7-one 444607-08-3P, N-[8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-7-oxo-7,8-dihydropyrido[2,3-d]pyrimidin-2-yl]-N-methylmethanesulfonamide 444607-09-4P, N-[4-(4-Fluoro-2-methylphenyl)-8-isopropyl-7-oxo-7,8-dihydropyrido[2,3-d]pyrimidin-2-yl]-N-methylmethanesulfonamide 444607-13-0P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-hydroxy-8H-pyrido[2,3-d]pyrimidin-7-one 444607-23-2P, 8-(2,6-Dimethylphenyl)-4-(4-fluoro-2-methylphenyl)-2-(2-hydroxyethylamino)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-24-3P, 8-(2,6-Dimethylphenyl)-4-(4-fluoro-2-methylphenyl)-2-[(2-hydroxy-1-hydroxymethylethyl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444607-25-4P, 4-(4-Fluoro-2-methylphenyl)-2-[(2-hydroxy-1-hydroxymethylethyl)amino]-8-(o-tolyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-26-5P, 4-(4-Fluoro-2-methylphenyl)-2-(2-hydroxyethylamino)-8-o-tolyl-8H-pyrido[2,3-d]pyrimidin-7-one 444607-28-7P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-(3-methanesulfonylpropoxy)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-29-8P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-(2-hydroxy-1-hydroxymethylethoxy)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-32-3P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-(2-acetylaminoethoxy)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-33-4P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-(3-hydroxy-2-hydroxymethylpropoxy)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-35-6P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-[2-(N-methanesulfonyl-N-methylamino)ethoxy]-8H-pyrido[2,3-d]pyrimidin-7-one 444607-36-7P, 4-(4-Fluoro-2-methylphenyl)-8-(2-fluorophenyl)-2-(2-hydroxyethylamino)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-37-8P, (S)-4-(4-Fluoro-2-methylphenyl)-8-(2,6-difluorophenyl)-2-[(1-hydroxyprop-2-yl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444607-38-9P, (R)-4-(4-Fluoro-2-methylphenyl)-8-(2,6-difluorophenyl)-2-[(1-hydroxyprop-2-yl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444607-39-0P, 4-(4-Fluoro-2-methylphenyl)-8-(2,6-difluorophenyl)-2-(1,1-dimethyl-2-hydroxyethylamino)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-40-3P, 2-Ethylamino-4-(4-fluoro-2-methylphenyl)-8-(2-fluorophenyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-41-4P, (S)-4-(4-Fluoro-2-methylphenyl)-8-(2-fluorophenyl)-2-[(1-hydroxyprop-2-yl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444607-42-5P, (R)-4-(4-Fluoro-2-methylphenyl)-8-(2-fluorophenyl)-2-[(1-hydroxyprop-2-

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 444608-16-6P, 4-(4-Fluoro-2-methylphenyl)-2-morpholin-4-yl-8-o-tolyl-8H-  
 pyrido[2,3-d]pyrimidin-7-one 444608-18-8P, 8-(2,6-Difluorophenyl)-4-(4-  
 fluoro-2-methylphenyl)-2-[[{(1SR,2SR)-2-hydroxycyclohexyl]amino]-8H-  
 pyrido[2,3-d]pyrimidin-7-one 444608-20-2P, 2-[[8-(2,6-Difluorophenyl)-4-  
 (4-fluoro-2-methylphenyl)-7-oxo-7,8-dihydropyrido[2,3-d]pyrimidin-2-  
 yl]amino]-N-(2-hydroxyethyl)acetamide 444608-22-4P, 8-(2,6-  
 Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-[[2-(1H-tetrazol-5-  
 yl)ethyl]amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444608-23-5P,  
 N-Cyclopropyl-2-[[8-(2,6-difluorophenyl)-4-(4-fluoro-2-methylphenyl)-7-oxo-  
 7,8-dihydropyrido[2,3-d]pyrimidin-2-yl]amino]acetamide 444608-25-7P,  
 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-[(1H-tetrazol-5-  
 ylmethyl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444608-28-0P,  
 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-[(1SR,2SR)-2-  
 hydroxycyclopentylamino]-8H-pyrido[2,3-d]pyrimidin-7-one 444608-30-4P,  
 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-(3-  
 methanesulfonylpropylamino)-8H-pyrido[2,3-d]pyrimidin-7-one  
 444608-31-5P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-[[2-oxo-  
 2-(3-oxopiperazin-1-yl)ethyl]amino]-8H-pyrido[2,3-d]pyrimidin-7-one  
 444608-32-6P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-[[5-  
 methyl-4H-[1,2,4]triazol-3-yl)methyl]amino]-8H-pyrido[2,3-d]pyrimidin-7-  
 one 444608-33-7P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-  
 [(1,1-dioxotetrahydro-1-thiophen-3-ylmethyl)amino]-8H-pyrido[2,3-  
 d]pyrimidin-7-one 444608-35-9P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-  
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 d]pyrimidin-7-one 444608-37-1P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-  
 methylphenyl)-2-[[{(3S,4S)-4-hydroxy-1,1-dioxotetrahydrothiophen-3-  
 yl]amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444608-39-3P,  
 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-[[2-oxo-2,3-  
 dihydropyrimidin-4-yl]amino]-8H-pyrido[2,3-d]pyrimidin-7-one  
 444608-40-6P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-[(1H-  
 imidazol-2-ylmethyl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444608-41-7P,  
 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-[(1H-[1,2,4]triazol-3-  
 yl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444608-42-8P,  
 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-(1H-tetrazol-5-  
 ylamino)-8H-pyrido[2,3-d]pyrimidin-7-one 444608-43-9P,  
 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-(2-methoxyethylamino)-  
 8H-pyrido[2,3-d]pyrimidin-7-one 444608-44-0P, 8-(2,6-Difluorophenyl)-4-  
 (4-fluoro-2-methylphenyl)-2-(tetrahydrofuran-3-ylamino)-8H-pyrido[2,3-  
 d]pyrimidin-7-one 444608-46-2P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-  
 methylphenyl)-2-[(2-hydroxyethyl)(methyl)amino]-8H-pyrido[2,3-d]pyrimidin-  
 7-one 444608-47-3P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-  
 [[2-(1H-imidazol-4-yl)ethyl]amino]-8H-pyrido[2,3-d]pyrimidin-7-one  
 444608-48-4P, 2-[[8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-7-oxo-  
 7,8-dihydropyrido[2,3-d]pyrimidine-2-ylamino]acetamide 444608-49-5P,  
 Cyclopropanecarboxylic acid [8-(2,6-difluorophenyl)-4-(4-fluoro-2-  
 methylphenyl)-7-oxo-7,8-dihydropyrido[2,3-d]pyrimidine-2-yl]amide  
 444608-51-9P, Cyclopropanecarboxylic acid (1-cyclopropylmethanoyl) [8-(2,6-  
 difluorophenyl)-4-(4-fluoro-2-methylphenyl)-7-oxo-7,8-dihydropyrido[2,3-  
 d]pyrimidin-2-yl]amide 444608-53-1P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-  
 2-methylphenyl)-2-[(tetrahydrofuran-2-ylmethyl)amino]-8H-pyrido[2,3-  
 d]pyrimidin-7-one 444608-54-2P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-  
 methylphenyl)-2-[[2-(3-hydroxyazetidin-1-yl)-2-oxoethyl]amino]-8H-  
 pyrido[2,3-d]pyrimidin-7-one 444608-55-3P, 4-(4-Fluoro-2-methylphenyl)-2-  
 ((R)-2-hydroxypropylamino)-8-o-tolyl-8H-pyrido[2,3-d]pyrimidin-7-one  
 444608-56-4P, 4-(4-Fluoro-2-methylphenyl)-2-(2-hydroxy-2-  
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 444608-57-5P, (1SR,2RS)-2-[[8-(2,6-Difluorophenyl)-4-(4-fluoro-2-  
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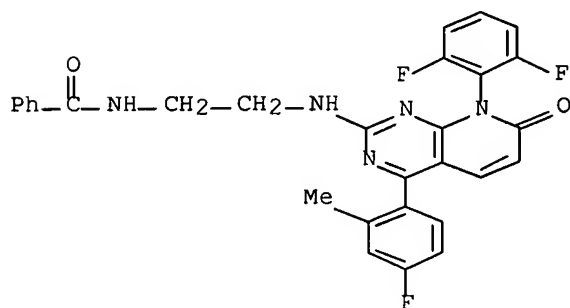
RN 444607-60-7 HCAPLUS

CN Urea, N-[2-[[8-(2,6-difluorophenyl)-4-(4-fluoro-2-methylphenyl)-7,8-dihydro-7-oxopyrido[2,3-d]pyrimidin-2-yl]amino]ethyl]-N'-(3-fluorophenyl)- (CA INDEX NAME)



RN 444607-62-9 HCAPLUS

CN Benzamide, N-[2-[[8-(2,6-difluorophenyl)-4-(4-fluoro-2-methylphenyl)-7,8-dihydro-7-oxopyrido[2,3-d]pyrimidin-2-yl]amino]ethyl]- (CA INDEX NAME)



L163 ANSWER 11 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:540257 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 137:109288

TITLE: Preparation of pyrrolo[2,3-d]pyrimidines as selective inhibitors of the adenosine A3 receptor

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan; Witter, David J.

AB Pyrrolopyrimidines I [R = 3-hydroxycyclopentylamino ethylamino carbonylamino Pr, N,N-diethylamino carbonylamino Et, thioacetamido Et, 3-amino acetyloxy cyclopentyl, 3-hydroxycyclopentyl, 2-pyrrolyl carbonyl aminoethyl, 2-imidazolinone Et, 1-aminocarbonyl-2-methylpropyl, 1-aminocarbonyl-2-Ph Et, 3-hydroxyazetidino, 2-imidazoleethyl, acetamidoethyl, 1-(R)-phenyl-2-hydroxyethyl, N-methylaminocarbonyl pyridyl-2-methyl; R1 = H; RR1N = 3-hydroxypyrrolidino, 3-methyloxy carbonylmethyl pyrrolidino, 3-aminocarbonylmethyl pyrrolidino, 3-hydroxymethyl piperidino; R3, R4 = H, (un)substituted alkyl, aryl] are prepared as selective inhibitors of adenosine receptors, particularly the adenosine A3 receptor, for the treatment of diseases such as asthma, diarrhea, chronic obstructive pulmonary disease, allergic rhinitis, or for the treatment of eye damage caused either by disease or injury. Human adenosine receptors are transformed into yeast; the modified yeast are used to assay the invention compds. I for their adenosine receptor binding and selectivities. E.g., 1-(1-phenylethyl)-2-amino-3-cyano-4,5-dimethylpyrrole is acylated with PhCOCl to give the benzamide which undergoes cyclocondensation with concentrated H2SO4 in MeOH to give a pyrrolopyrimidinone; removal of the phenethyl group with polyphosphoric acid and chlorination of the pyrrolopyrimidinone with POCl3 gives the intermediate chloropyrrolopyrimidine II. E.g., addition of amines such as trans-3-amino-1-cyclopentanol to II in DMSO gives aminopyrrolopyrimidines such as III. III has a Ki for the adenosine A1 receptor of 29 nM and a Ki for the adenosine A3 receptor of 3.1 nM while binding to the adenosine A2a and A2b receptors with Ki values of 191 nM and 1143 nM, resp. Formulations of these compds. are claimed (no data). Methods for the preparation of I from the acylation of aminopyrroles with acyl chlorides followed by cyclocondensation and deprotection, chlorination, and substitution of the chlorine atom with an amine are claimed.

IC ICM A61K031-519

ICS C07D487-04

INCL 514210210

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 63

IT Allergy

Arthritis

Asthma

Autoimmune disease

Carcinoma

Cardiovascular system, disease

Central nervous system, disease

Cognitive disorders

Dermatitis

Diabetes insipidus

Diabetes mellitus

Diarrhea

Digestive tract, disease

Diuresis

Eczema

Edema

Eye, disease

Glaucoma (disease)

Granulomatous disease

Graves' disease

Hay fever

Hypertension

Immune disease

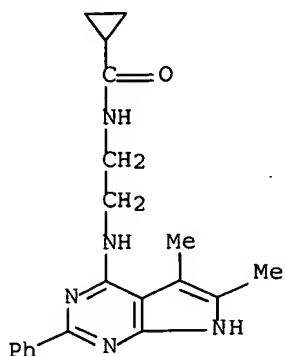
Inflammation

Kidney, disease

injuries or disease)

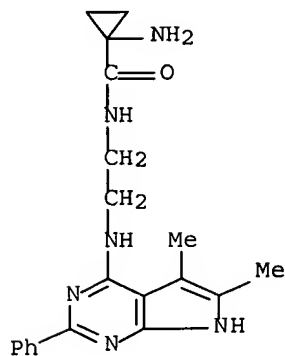
RN 251946-27-7 HCAPLUS

CN Cyclopropanecarboxamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)



RN 343632-15-5 HCAPLUS

CN Cyclopropanecarboxamide, 1-amino-N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)



RN 343632-38-2 HCAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[2-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2806082	A1	20010914	FR 2000-2902	20000307 <--
FR 2806082	B1	20020517		
CA 2402686	A1	20011025	CA 2001-2402686	20010306 <--
WO 2001079172	A1	20011025	WO 2001-FR650	20010306 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
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BR 2001008998	A	20021217	BR 2001-8998	20010306 <--
EP 1268429	A1	20030102	EP 2001-969041	20010306 <--
EP 1268429	B1	20040818		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
HU 2003000181	A2	20030528	HU 2003-181	20010306 <--
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JP 3974780	B2	20070912		
AT 273957	T	20040915	AT 2001-969041	20010306 <--
PT 1268429	T	20041029	PT 2001-969041	20010306 <--
NZ 520805	A	20041224	NZ 2001-520805	20010306 <--
ES 2227265	T3	20050401	ES 2001-1969041	20010306 <--
ZA 2002006354	A	20030808	ZA 2002-6354	20020808 <--
MX 2002PA08633	A	20030224	MX 2002-PA8633	20020903 <--
US 2003229109	A1	20031211	US 2002-220755	20020903 <--
US 6846833	B2	20050125		
NO 2002004275	A	20020906	NO 2002-4275	20020906 <--
NO 324052	B1	20070806		
HK 1052345	A1	20051230	HK 2003-104528	20030624 <--
PRIORITY APPLN. INFO.:			FR 2000-2902	A 20000307 <--
			WO 2001-FR650	W 20010306
OTHER SOURCE(S):		MARPAT 137:63182		
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I, including enantiomers, diastereoisomers, and pharmaceutically acceptable acid and base addition salts, are disclosed [wherein: G = C, CH, N, or O, forming a benzene or aromatic or partially unsatd. heterocyclic group containing 1-2 heteroatoms and optionally substituted by R1-R4; G1, G2 = C or N; R1-R4 = halo, alkyl, perhaloalkyl, cyano, NO2, OR7, NR6R6', CO2R6, CONR6R6', COR6, S(O)nR6, or absent; n = 0-2; T1 = CH2CH2, CH:CH, :CHCH2 and T2 = bond; or T1 = CH2 or :CH and T2 = CH2 or :CH; R5 = (CH2)mCOOR6; R6, R6' = H, alkyl, (un)substituted aryl or arylalkyl; R7 = H, alkyl; W = CH, :C, or C: and A = CO, CH, :CH, or CH:; or W = N and A = CO or CH2; X = COX1, CONR6X1, NR6COX1, OX1, SO2NR6X1, S(O)nX1; X1 = alkylene; Y = Y1, Y2Y1, Y1Y2Y1; Y1 = alkylene, alkenylene, or alkynylene; Y2 = arylene, heteroarylene, cycloalkylene, or heterocycloalkylene; Z = Z1, Z10NR6, or Z10NR6CO; Z10 = alkyl or Z1; Z1 = Z2, Z20C(:NR6), Z20NR6, and Z20NR6CO; Z20 = alkyl, heteroalkyl, or Z2; Z2 = (un)substituted heteroaryl, heterocycloalkyl, heteroarylheteroalkyl, heterocycloalkylalkyl, fused arylheteroaryl, fused arylheterocycloalkyl, fused heteroarylheterocycloalkyl, fused heteroarylheteroaryl, or fused cycloalkylheterocycloalkyl; m = 1-6]. Approx.



## vitronectin receptor antagonists)

IT 439609-07-1P, [7-[[[5-(2-Pyridinylamino)pentyl]oxy)methyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetic acid hydrochloride 439609-09-3P, [7-[[[4-(2-Pyridinylamino)butyl]oxy)methyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetic acid hydrochloride 439609-11-7P, [7-[[[3-(2-Pyridinylamino)propyl]oxy)methyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetic acid hydrochloride 439609-12-8P, [7-[[[3-[(2-Pyridinylamino)methyl]benzyl]oxy)methyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetic acid hydrochloride 439609-13-9P, [7-[2-Oxo-2-[[3-(2-pyridinylamino)propyl]amino]ethyl]-5H-benzocyclohepten-5-yl]acetic acid 439609-14-0P, [7-[2-Oxo-2-[[3-(2-pyridinylamino)propyl]amino]ethyl]-5H-benzocyclohepten-5-yl]acetic acid trifluoroacetate 439609-16-2P, [7-[2-Oxo-2-[[4-(2-pyridinylamino)butyl]amino]ethyl]-5H-benzocyclohepten-5-yl]acetic acid trifluoroacetate 439609-18-4P, [7-[2-Oxo-2-[[2-(2-pyridinylamino)ethyl]amino]ethyl]-5H-benzocyclohepten-5-yl]acetic acid trifluoroacetate 439609-20-8P, [7-[2-Oxo-2-[[3-[(2-pyridinylamino)methyl]benzyl]amino]ethyl]-5H-benzocyclohepten-5-yl]acetic acid trifluoroacetate 439609-22-0P, [7-[2-Oxo-2-[[3-[N-(4,5,6,7-tetrahydro-3H-azepin-2-yl)amino]propyl]amino]ethyl]-5H-benzocyclohepten-5-yl]acetic acid trifluoroacetate 439609-24-2P, [7-[2-Oxo-2-[[3-[(4,5-dihydro-1H-imidazol-2-yl)amino]propyl]amino]ethyl]-5H-benzocyclohepten-5-yl]acetic acid trifluoroacetate 439609-26-4P, [7-[2-Oxo-2-[[3-[(4,5-dihydro-1H-imidazol-2-ylamino)methyl]benzyl]amino]ethyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetic acid trifluoroacetate 439609-27-5P, [7-[[[4-(2-Pyridinylamino)butanoyl]amino]methyl]-5H-benzocyclohepten-5-yl]acetic acid 439609-28-6P, [7-[[[4-(2-Pyridinylamino)butanoyl]amino]methyl]-5H-benzocyclohepten-5-yl]acetic acid trifluoroacetate 439609-30-0P, [7-[[[5-(2-Pyridinylamino)pentanoyl]amino]methyl]-5H-benzocyclohepten-5-yl]acetic acid trifluoroacetate 439609-32-2P, [7-[[[4-[(3,4,5,6-Tetrahydro-2H-azepin-7-yl)amino]butanoyl]amino]methyl]-5H-benzocyclohepten-5-yl]acetic acid trifluoroacetate 439609-34-4P, [7-[[[5-[(3,4,5,6-Tetrahydro-2H-azepin-7-yl)amino]pentanoyl]amino]methyl]-5H-benzocyclohepten-5-yl]acetic acid trifluoroacetate 439609-36-6P, [7-[[[4-[(4,5-Dihydro-1H-imidazol-2-yl)amino]butanoyl]amino]methyl]-5H-benzocyclohepten-5-yl]acetic acid trifluoroacetate 439609-38-8P, [7-[[[5-[(4,5-Dihydro-1H-imidazol-2-yl)amino]pentanoyl]amino]methyl]-5H-benzocyclohepten-5-yl]acetic acid trifluoroacetate 439609-39-9P, [7-[[[4-(1H-Benzimidazol-2-ylamino)butanoyl]amino]methyl]-5H-benzocyclohepten-5-yl]acetic acid 439609-40-2P, [7-[[[4-(1H-Benzimidazol-2-ylamino)butanoyl]amino]methyl]-5H-benzocyclohepten-5-yl]acetic acid trifluoroacetate 439609-42-4P, [7-[[[5-(1H-Benzimidazol-2-ylamino)pentanoyl]amino]methyl]-5H-benzocyclohepten-5-yl]acetic acid trifluoroacetate 439609-44-6P, [7-[[[3-(2-Pyridinylamino)propanoyl]amino]methyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetic acid trifluoroacetate 439609-45-7P, [7-[[[4-(2-Pyridinylamino)butanoyl]amino]methyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetic acid hydrochloride 439609-46-8P, [7-[[[5-(2-Pyridinylamino)pentanoyl]amino]methyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetic acid hydrochloride 439609-49-1P, [7-[[[3-[(2-Pyridinylamino)methyl]benzoyl]amino]methyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetic acid trifluoroacetate 439609-50-4P, [7-[[[4-(1H-Benzimidazol-2-ylamino)butanoyl]amino]methyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetic acid hydrochloride 439609-52-6P, [7-[[[4-[(N1-4,5,6,7-Tetrahydro-3H-azepin-2-yl)amino]butanoyl]amino]methyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetic acid hydrochloride 439609-54-8P, [7-[[[4-[(4,5-Dihydro-1H-imidazol-2-yl)amino]butanoyl]amino]methyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetic acid hydrochloride 439609-57-1P, [7-[[[3-[(1,4,5,6-Tetrahydro-2-pyrimidinyl)amino]methyl]benzoyl]amino]methyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetic acid trifluoroacetate 439609-60-6P,

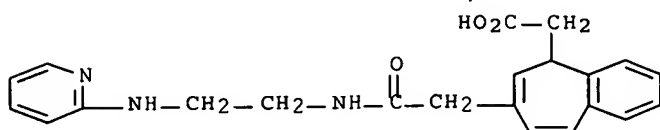
RN 439609-18-4 HCAPLUS

CN 5H-Benzocycloheptene-5-acetic acid, 7-[2-oxo-2-[[2-(2-pyridinylamino)ethyl]amino]ethyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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CRN 439609-17-3

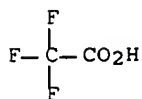
CMF C22 H23 N3 O3



CM 2

CRN 76-05-1

CMF C2 H F3 O2



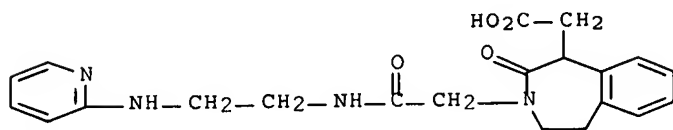
RN 439609-66-2 HCAPLUS

CN 1H-3-Benzazepine-1-acetic acid, 2,3,4,5-tetrahydro-2-oxo-3-[2-oxo-2-[[2-(2-pyridinylamino)ethyl]amino]ethyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 439609-65-1

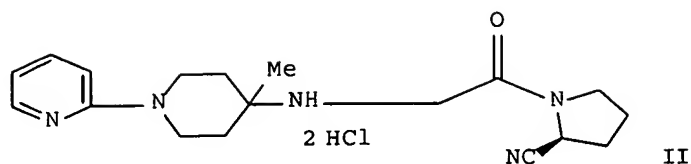
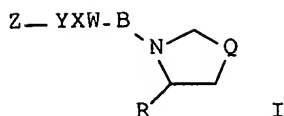
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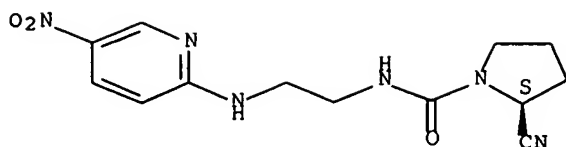
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CRN 76-05-1

CMF C2 H F3 O2



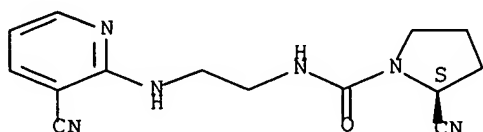
- AB Title compds. [I; Q = CH<sub>2</sub>, S; R = H, (S)-CN; B = CH<sub>2</sub>CO, COCH<sub>2</sub>, CO; YXW = NHCH<sub>2</sub>CH<sub>2</sub>NH, NH(CH<sub>2</sub>)<sub>3</sub>NH, NHCH<sub>2</sub>C(CH<sub>3</sub>)<sub>2</sub>NH, 1-(4-methyl-piperidine-4-amino)-yl, 1-(1-aminomethylcyclopropyl)amino, 4-NHCH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>NH, N(CH<sub>3</sub>)CH<sub>2</sub>CH<sub>2</sub>N(CH<sub>3</sub>), 1,4-piperazinyl, 1-piperidinyl-4-amino, N(CH<sub>3</sub>)CH<sub>2</sub>C(CH<sub>3</sub>)<sub>2</sub>NH; Z = optionally substituted 1-pyrrolidinyl, optionally substituted 3-thiazolidinyl, optionally substituted 1-oxo-3-thiozolidinyl, etc.] and pharmacol. acceptable salts of title compds. are prepared as dipeptidyl peptidase IV inhibitors. Title compds. are useful as antidiabetics, antiaids agents, antiarteriosclerosis, antihyperglycinemia agents, and as remedies for hyperglycinemia, hyperinsulinism, etc. in combination with related remedies as GI-262570, KAD1229, etc. Thus, the title compound II was prepared and in vivo tested for DPP-IV inhibition with IC<sub>50</sub> = 11 nmol/L.
- IC ICM C07D401-12  
ICS C07D417-12; C07D401-14; C07D403-12; C07D405-12; C07D207-16;  
C07D417-14; A61K031-4709; A61K031-4725; A61K031-428; A61K031-4439;  
A61K031-496; A61K031-4545; A61K031-497; A61K031-498; A61K031-506;  
A61K031-433; A61K031-502; A61K031-501; A61K031-5377
- CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1, 63
- IT AIDS (disease)  
Anorexia  
Anti-AIDS agents  
Antiarthritics  
Antidiabetic agents  
Arteriosclerosis  
Arthritis  
Autoimmune disease  
Fertility disorders  
Human  
Osteoporosis  
Substitution reaction  
(preparation of aminocarbonylpyrrolidine derivs. as dipeptidyl peptidase IV inhibitors)
- |    |              |              |              |              |              |
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|    | 440099-68-3P | 440099-70-7P | 440099-71-8P | 440099-73-0P | 440099-75-2P |
|    | 440099-77-4P | 440099-78-5P | 440099-79-6P | 440099-80-9P | 440099-81-0P |
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RN 440101-07-5 HCAPLUS

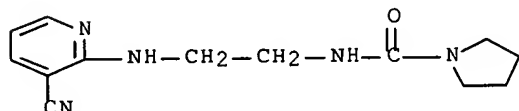
CN 1-Pyrrolidinecarboxamide, 2-cyano-N-[2-[(3-cyano-2-pyridinyl)amino]ethyl] -  
, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 440101-08-6 HCAPLUS

CN 1-Pyrrolidinecarboxamide, N-[2-[(3-cyano-2-pyridinyl)amino]ethyl] - (CA  
INDEX NAME)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 14 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:487561 HCAPLUS Full-text

DOCUMENT NUMBER: 137:63240

TITLE: Preparation of thiazolyl inhibitors of Tec family  
tyrosine kinases

INVENTOR(S): Barrish, Joel C.; Das, Jagabandhu; Kanner, Steven B.;  
Liu, Chunjian; Spergel, Steven H.; Witayk, John;  
Doweyko, Arthur M. P.; Furch, Joseph A.

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: PCT Int. Appl., 149 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002050071	A1	20020627	WO 2001-US49430	20011219 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,				

AB The title compds. [I; Q1 = thiazolyl; Q2 = (un)substituted (hetero)aryl; Z = O, S, NR4, etc.; R1 = H, OH, SH, etc.; R2, R3 = H, (un)substituted (hetero)aryl, (hetero)arylcarbonyl, etc.; R4 = H, alkyl, aryl, etc.], useful in the treatment of Tec family tyrosine kinase-associated disorders such as cancer, immunol. disorders and allergic disorders, were prepared E.g., a multi-step synthesis of the thiazole II, was given.

IC ICM C07D417-12  
ICS C07D417-14; A61P029-00

CC 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1

IT Nervous system, disease  
(Guillain-Barre syndrome; preparation of thiazolyl inhibitors of Tec family tyrosine kinases)

IT Allergy  
Allergy inhibitors  
Anti-inflammatory agents  
Antiasthmatics  
Antirheumatic agents  
Antitumor agents  
Asthma  
Human  
Immunosuppressants  
Lupus erythematosus  
Multiple sclerosis  
Neoplasm  
Psoriasis  
Rheumatoid arthritis  
Transplant rejection  
(preparation of thiazolyl inhibitors of Tec family tyrosine kinases)

IT

439576-67-7P	439576-68-8P	439576-69-9P	439576-70-2P	439576-71-3P
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OTHER SOURCE(S):      MARPAT 136:340677
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of imidazoarene prostaglandin EP4 receptor antagonists as antiinflammatory and analgesic agents)

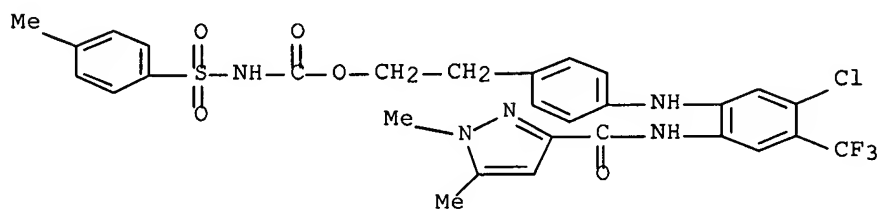
IT 415911-73-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of imidazoarene prostaglandin EP4 receptor antagonists as antiinflammatory and analgesic agents)

RN 415911-73-8 HCAPLUS

CN Carbamic acid, [(4-methylphenyl)sulfonyl]-, 2-[4-[[5-chloro-2-[[[(1,5-dimethyl-1H-pyrazol-3-yl)carbonyl]amino]-4-(trifluoromethyl)phenyl]amino]phenyl]ethyl ester (9CI) (CA INDEX NAME)



L163 ANSWER 16 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:314767 HCAPLUS Full-text

DOCUMENT NUMBER: 136:340676

TITLE: Preparation of benzimidazole derivatives as prostaglandin EP4 receptor inhibitors to treat rheumatoid arthritis

INVENTOR(S): Audoly, Laurent; Okumura, Takako; Shimojo, Masato

PATENT ASSIGNEE(S): Pfizer Pharmaceuticals Inc., Japan; Pfizer Inc.

SOURCE: PCT Int. Appl., 468 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

AB Benzimidazole derivs. I wherein Y1-Y4 are independently N, CH, alkyl, alkoxy, haloalkyl, halo, substituted alkyl, R1 is H, alkyl, alkenyl, alkynyl, cycloalkyl, alkoxy, haloalkoxy, heterocycle; R2 is H, alkyl, alkoxy, OH; A is substituted heterocycle arom ring; B is haloalkylene, cycloalkylene, alkenylene, alkynylene, oxyalkylene; W is NH, aminoalkyl, O, S, oxime, covalent bond; Z is monocyclic and bicyclic aromatic heterocycle, were prepared as prostaglandin EP4 receptor inhibitors to treat rheumatoid arthritis of rats and human. Also featured is a method of identifying agents that selectively inhibit EP4 activity in vivo. Thus, 3-(4-{2[{[(3,4-dichlorophenyl)sulfonyl]amino}carbonyl]amino}ethyl}phenyl)-2-ethyl-5,7-dimethyl-3H-imidazo[4,5-b]pyridine, hydrochloride was prepared and tested in vivo as an agent selectively inhibiting EP4 activity or selectively binding EP4; and measuring joint inflammation, joint swelling, joint ankylosis, interleukin (IL)-6, SAA protein, and/or joint mobility.

IC ICM A61K031-4178  
ICS A61K031-437; A61P029-00; A61K031-64

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1, 63

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(trifluoromethyl)phenyl]amino]phenyl)-2-propanol 415911-83-0P,  
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(2S)-1-(4-Aminophenyl)-2-propanol 415911-89-6P, 1-[4-((4-[(2S)-2-  
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(2R)-1-(4-Aminophenyl)-2-propanol 415911-97-6P, 1-[4-((4-[(2R)-2-  
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415912-33-3P 415912-34-4P 415912-35-5P 415912-36-6P, Diethyl  
2-(2-chloro-4-nitrophenyl)malonate 415912-37-7P, Methyl



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 415913-91-6P, 1,5-Dichloro-2-[(methoxy)methyl]-4-nitrobenzene 415913-92-7P, 2-[4-([5-Chloro-4-[(methoxy)methyl]-2-nitrophenyl]amino)phenyl]ethanol 415913-93-8P, 2-[4-([2-Amino-5-chloro-4-[(methoxy)methyl]phenyl]amino)phenyl]ethanol 415913-94-9P 415913-95-0P  
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 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of benzimidazole derivs. as prostaglandin ep receptor inhibitors to treat rheumatoid arthritis)

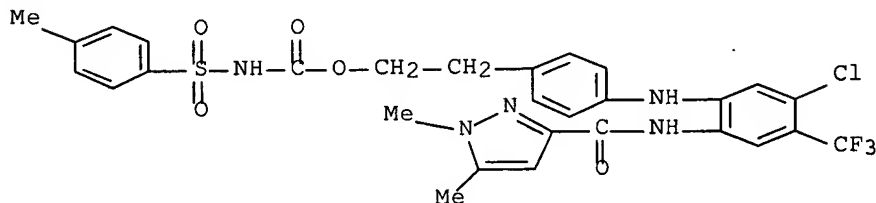
IT 415911-73-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of benzimidazole derivs. as prostaglandin ep receptor inhibitors to treat rheumatoid arthritis)

RN 415911-73-8 HCAPLUS

CN Carbamic acid, [(4-methylphenyl)sulfonyl]-, 2-[4-[[5-chloro-2-[[[1,5-dimethyl-1H-pyrazol-3-yl]carbonyl]amino]-4-(trifluoromethyl)phenyl]amino]phenyl]ethyl ester (9CI) (CA INDEX NAME)



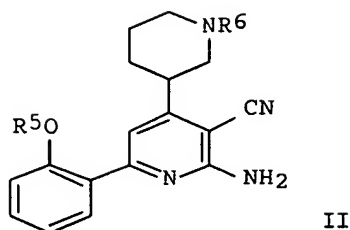
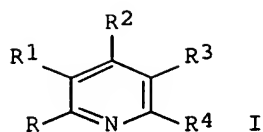
L163 ANSWER 17 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:240756 HCAPLUS Full-text

DOCUMENT NUMBER: 136:279345

TITLE: Preparation of hydroxyarylpyridines with IkB kinase  $\beta$  (IKK) inhibiting activity

INVENTOR(S): Lowinger, Timothy B.; Murata, Toshiki; Umeda, Masaomi;



AB Pyridines I [R = 3-hydroxy-2-pyridyl, 3-hydroxy-2-thienyl, (substituted)-2-hydroxyphenyl; R1 = H, halogen; R2 = H, 1,2,3,6-tetrahydropyridyl, (un)substituted amino, etc.; R3 = HO2C, alkylcarbonyl, alkylcarbamoyl, alkylamino, (heteroaryl)hydroxymethyl, (heteroaryl)alkyl, etc.; R4 = (un)substituted amino; R2 and R3 or R3 and R4 may form fused cycloalkyl or bicycloalkyl moieties optionally containing NH moieties] such as II.HCl were prepared as IκB kinase β (IKK) inhibitors for the inhibition of nuclear factor κB (NF-κB) activity and the treatment of inflammatory diseases, such as asthma and ischemia; in addition, the compds. are antitumor and immunosuppressant agents. E.g., 2'-benzyloxyacetophenone, tert-Bu 3-formyl-1-piperidinecarboxylate, and malononitrile were stirred with NH4OAc in PhMe at 150° to yield aminopyridine II (R5 = PhCH2; R6 = Me3COCO) in 27% yield; removal of the benzyl group with Pd/C followed by removal of the Boc group with HCl in dioxane yielded the monohydrochloride of II (R5 = R6 = H) which showed good in vitro and cellular activities. Over 300 examples are prepared with biol. data.

IC ICM C07D401-04

ICS C07D213-85; C07D401-14; C07D409-14; C07D401-06; C07D413-14;  
C07D405-14; C07D471-04; A61P017-00; A61P011-06; A61P029-00;  
A61K031-4427; A61K031-4353; C07D471-18; C07D498-04; C07D213-80;  
C07D213-73; C07D521-00; C07D513-04

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1

IT Dermatomyositis

Gout

Psoriasis

Rheumatoid arthritis

Sepsis

Sjogren syndrome

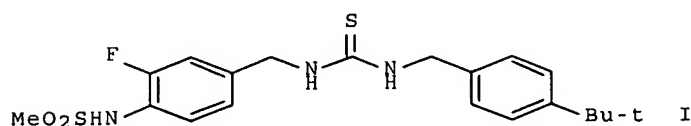
Urticaria

(treatment; preparation of (hydroxyaryl)pyridines as inhibitors of IκB kinase β and as antiinflammatory, immunosuppressant, antitumor, and antiischemic agents)

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	406211-71-0P	406211-72-1P	406211-73-2P	406211-74-3P	406211-75-4P

vanilloid receptor (VR)  
 INVENTOR(S): Suh, Young Ger; Oh, Uh Taek; Kim, Hee Doo; Lee, Jee Woo; Park, Hyeung Geun; Park, Ok Hui; Lee, Yong Sil; Park, Young Ho; Joo, Yung Hyup; Choi, Jin Kyu; Lim, Kyung Min; Kim, Sun Young; Kim, Jin Kwan; Koh, Hyun Ju; Moh, Joo Hyun; Jeong, Yeon Su; Yi, Jung Bum; Oh, Young Im  
 PATENT ASSIGNEE(S): Pacific Corporation, S. Korea  
 SOURCE: PCT Int. Appl., 245 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002016318	A1	20020228	WO 2001-KR1407	20010820 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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AU 200180229	A	20020304	AU 2001-80229	20010820 <--
KR 2002039226	A	20020525	KR 2001-50092	20010820 <--
EP 1303483	A1	20030423	EP 2001-958602	20010820 <--
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NZ 523882	A	20041126	NZ 2001-523882	20010820 <--
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MX 2003PA01535	A	20041213	MX 2003-PA1535	20030220 <--
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PRIORITY APPLN. INFO.:			KR 2000-48385	A 20000821 <--
			KR 2000-48388	A 20000821 <--
			KR 2000-85126	A 20001229 <--
			KR 2001-50092	A3 20010820
			KR 2001-50093	A3 20010820
			WO 2001-KR1407	W 20010820
			KR 2004-32384	A3 20040507
OTHER SOURCE(S):			MARPAT 136:216541	
GI				



401908-42-7P 401908-43-8P 401908-44-9P 401908-45-0P 401908-46-1P  
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation);  
 THU (Therapeutic use); BIOL (Biological study); PREP  
 (Preparation); USES (Uses)

(preparation of novel thioureas as modulators for vanilloid receptor (VR))

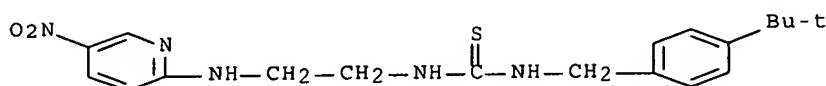
IT 401908-28-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);  
 THU (Therapeutic use); BIOL (Biological study); PREP  
 (Preparation); USES (Uses)

(preparation of novel thioureas as modulators for vanilloid receptor (VR))

RN 401908-28-9 HCAPLUS

CN Thiourea, N-[[4-(1,1-dimethylethyl)phenyl)methyl]-N'-[2-[(5-nitro-2-pyridinyl)amino]ethyl]- (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 19 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:107321 HCAPLUS Full-text

DOCUMENT NUMBER: 136:167373

TITLE: Preparation of imidazolyl derivatives as agonists or antagonists of somatostatin receptors

INVENTOR(S): Thurieau, Christophe Alain; Poitout, Lydie Francine; Galcera, Marie-Odile; Gordon, Thomas D.; Morgan, Barry A.; Moinet, Christophe Philippe; Bigg, Dennis

PATENT ASSIGNEE(S): Societe De Conseils De Recherches Et D'applications Scientifiques (S.C.R.A.S.), Fr.

SOURCE: PCT Int. Appl., 369 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002010140	A2	20020207	WO 2001-US23959	20010731 <--
WO 2002010140	A3	20020808		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

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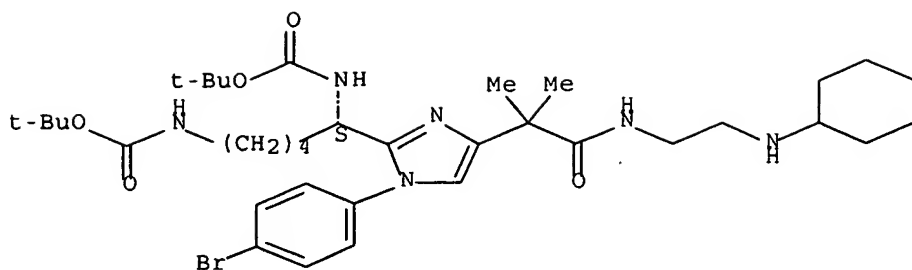
RL: PAC (Pharmacological activity); SPN (Synthetic preparation);

THU (Therapeutic use); BIOL (Biological study); PREP

(Preparation); USES (Uses)

(preparation of imidazolyl derivs. as agonists or antagonists of somatostatin receptors)

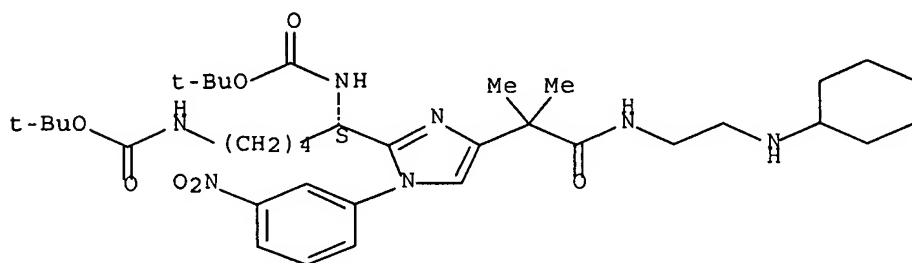
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RN 252295-88-8 HCAPLUS

CN Carbamic acid, [(1S)-1-[4-[2-[[2-(cyclohexylamino)ethyl]amino]-1,1-dimethyl-2-oxoethyl]-1-(3-nitrophenyl)-1H-imidazol-2-yl]-1,5-pentanedyl]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

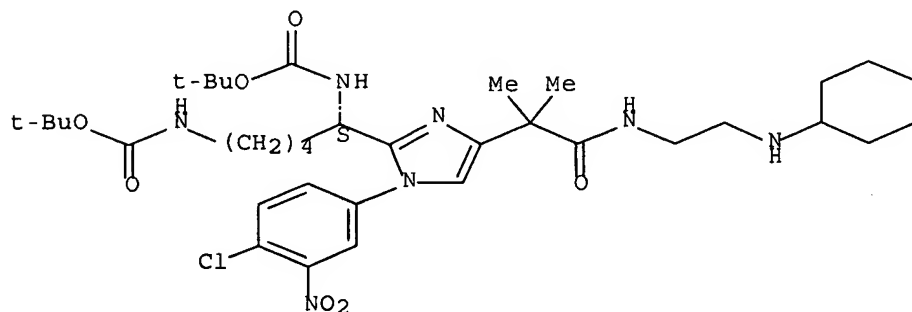
Absolute stereochemistry.



RN 252295-89-9 HCAPLUS

CN Carbamic acid, [(1S)-1-[1-(4-chloro-3-nitrophenyl)-4-[2-[[2-(cyclohexylamino)ethyl]amino]-1,1-dimethyl-2-oxoethyl]-1H-imidazol-2-yl]-1,5-pentanedyl]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

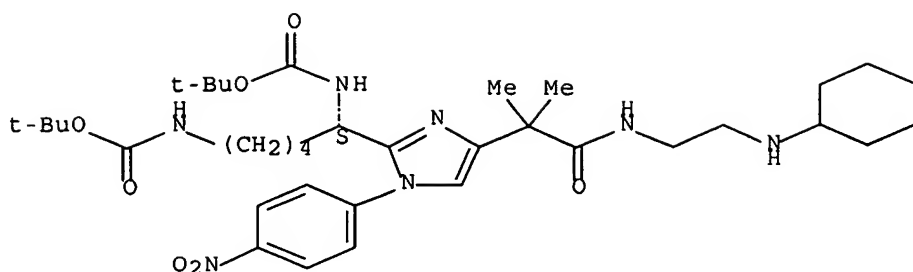
Absolute stereochemistry.



RN 252295-90-2 HCAPLUS

CN Carbamic acid, [(1S)-1-[4-[2-[[2-(cyclohexylamino)ethyl]amino]-1,1-dimethyl-2-oxoethyl]-1-(2-phenylethyl)-1H-imidazol-2-yl]-1,5-pentanedyl]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

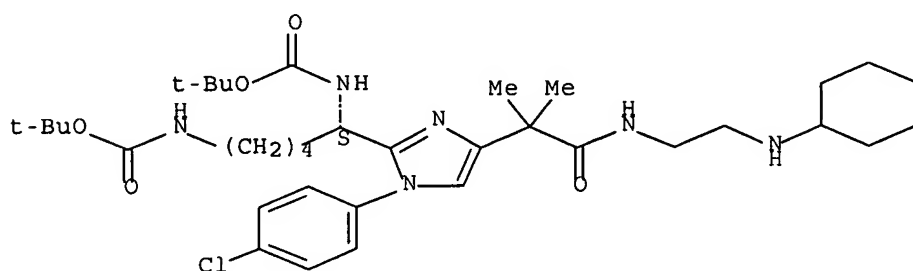
Absolute stereochemistry.



RN 252295-94-6 HCAPLUS

CN Carbamic acid, [(1S)-1-[1-(4-chlorophenyl)-4-[2-[[2-(cyclohexylamino)ethyl]amino]-1,1-dimethyl-2-oxoethyl]-1H-imidazol-2-yl]-1,5-pentanedyl]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

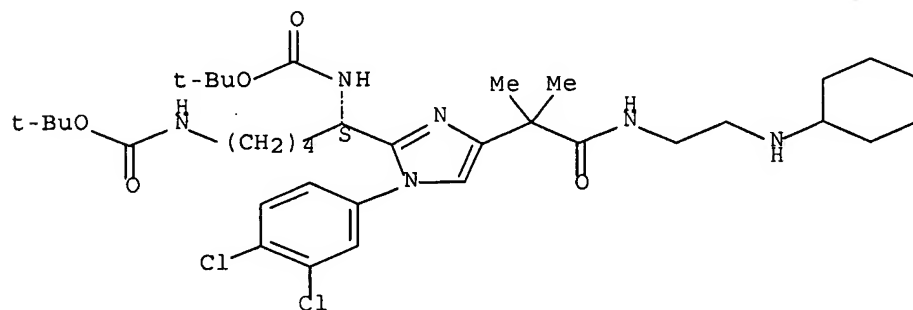
Absolute stereochemistry.



RN 252295-95-7 HCAPLUS

CN Carbamic acid, [(1S)-1-[4-[2-[[2-(cyclohexylamino)ethyl]amino]-1,1-dimethyl-2-oxoethyl]-1-(3,4-dichlorophenyl)-1H-imidazol-2-yl]-1,5-pentanedyl]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

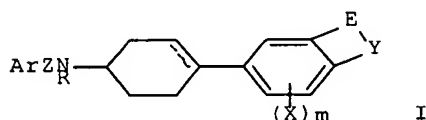


RN 252295-96-8 HCAPLUS

CN Carbamic acid, [(1S)-1-[4-[2-[[2-(cyclohexylamino)ethyl]amino]-1,1-dimethyl-2-oxoethyl]-1-(2,3-dihydro-1,4-benzodioxin-6-yl)-1H-imidazol-2-yl]-1,5-pentanedyl]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

EP 1286975	A1	20030305	EP 2001-933173	20010508 <--
EP 1286975	B1	20050824		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001011301	A	20030610	BR 2001-11301	20010508 <--
HU 2003002323	A2	20031028	HU 2003-2323	20010508 <--
JP 2003535083	T	20031125	JP 2002-500853	20010508 <--
EE 200200667	A	20040615	EE 2002-667	20010508 <--
AT 302763	T	20050915	AT 2001-933173	20010508 <--
ES 2245985	T3	20060201	ES 2001-1933173	20010508 <--
US 2003236252	A1	20031225	US 2002-276054	20021112
US 6794402	B2	20040921		
ZA 2002009325	A	20040216	ZA 2002-9325	20021115 <--
IN 2002MN01628	A	20041211	IN 2002-MN1628	20021115 <--
NO 2002005762	A	20030109	NO 2002-5762	20021129 <--
MX 2002PA11926	A	20030422	MX 2002-PA11926	20021129 <--
BG 107375	A	20030930	BG 2002-107375	20021211 <--
PRIORITY APPLN. INFO.:			US 2000-208241P	P 20000531 <--
			WO 2001-US14763	W 20010508
OTHER SOURCE(S): MARPAT 136:20063				
GI				

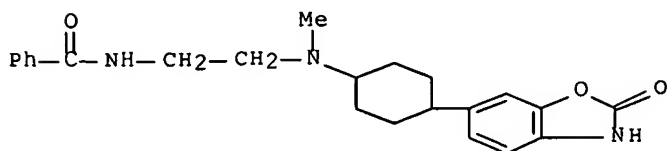


- AB Title compds. [I; Ar = (substituted) aryl, heteroaryl; Z = (CR<sub>1</sub>R<sub>2</sub>)<sub>n</sub>, O<sub>2</sub>C, OSO<sub>2</sub>, etc.; n = 1-6; R = H, alkyl, COR<sub>6</sub>, CO<sub>2</sub>R<sub>6</sub>, CONHR<sub>6</sub>, aralkyl, hydroxyalkyl, aminoalkyl, etc.; R<sub>6</sub> = alkyl, aralkyl; X = H, electron withdrawing group; m = 0-2; EY = CH:CHNH, CH<sub>2</sub>CH<sub>2</sub>NH, O<sub>2</sub>CNH, SCONH, N:NNH, CH:CHNH, N:CHNH, etc.; dotted line = optional double bond], were prepared Thus, a mixture of 6-(4-oxocyclohexyl)benzoxazolin-2-one (preparation given), Ph(CH<sub>2</sub>)<sub>3</sub>NH<sub>2</sub>, and 3A mol. sieves were stirred 4 h in Me<sub>2</sub>CHOH; NaBH<sub>4</sub> was added followed by stirring overnight to give 42% 6-[trans-4-(3-phenylpropylamino)cyclohexyl]-3H-benzoxazol-2-one (II). II inhibited NR1A/NR2B receptors in oocytes with IC<sub>50</sub> = 0.03 μM. A II drug formulation is given.
- IC ICM C07D263-58  
ICS C07D277-68; C07D235-26; C07D413-12; C07D417-12; A61K031-423; A61K031-428; A61K031-4184; A61P025-16
- CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1, 63
- IT Analgesics  
Anticonvulsants  
Antidepressants  
Antiglaucoma agents  
Antimigraine agents  
Antiparkinsonian agents  
Antipsychotics  
Anxiolytics  
(preparation of aminocyclohexylbenzazolinones as NMDA receptor antagonists)
- IT 377082-66-1P 377082-69-4P 377082-71-8P 377082-75-2P 377082-76-3P  
377082-81-0P 377082-87-6P 377082-89-8P 377082-92-3P 377082-96-7P  
377083-11-9P 377083-13-1P 377083-15-3P 377083-18-6P 377083-20-0P  
377083-25-5P 377083-27-7P 377083-29-9P 377083-31-3P 377083-33-5P



RN 377083-45-9 HCAPLUS

CN Benzamide, N-[2-[[4-(2,3-dihydro-2-oxo-6-benzoxazolyl)cyclohexyl]methylamino]ethyl]- (CA INDEX NAME)



IT 377083-46-0P 377085-55-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);

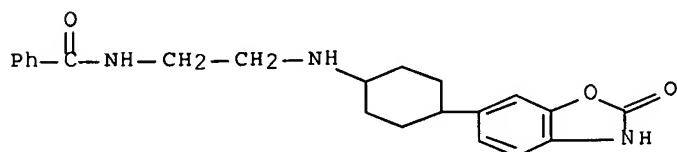
THU (Therapeutic use); BIOL (Biological study); PREP

(Preparation); USES (Uses)

(preparation of aminocyclohexylbenzazolones as NMDA receptor antagonists)

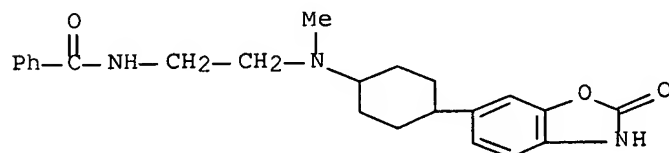
RN 377083-46-0 HCAPLUS

CN Benzamide, N-[2-[[4-(2,3-dihydro-2-oxo-6-benzoxazolyl)cyclohexyl]amino]ethyl]- (CA INDEX NAME)



RN 377085-55-7 HCAPLUS

CN Benzamide, N-[2-[[4-(2,3-dihydro-2-oxo-6-benzoxazolyl)cyclohexyl]methylamino]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

IT 377083-61-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of aminocyclohexylbenzazolones as NMDA receptor antagonists)

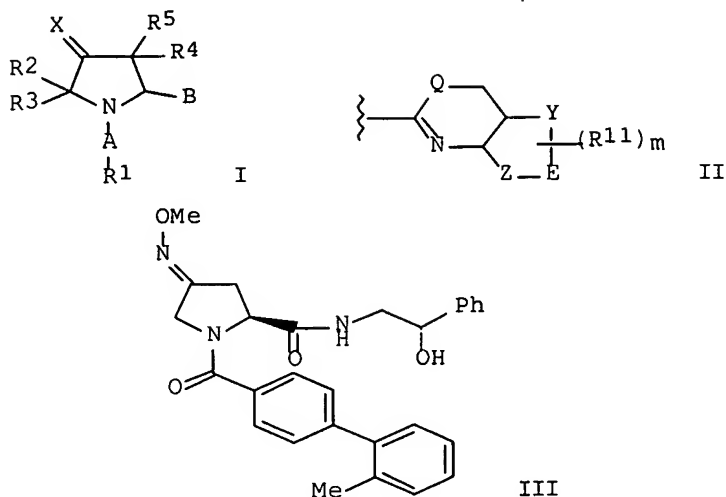
RN 377083-61-9 HCAPLUS

CN Benzamide, N-[2-[[4-(2,3-dihydro-2-oxo-6-benzoxazolyl)cyclohexyl]amino]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

NO 323969	B1	20070723		
MX 2002PA09382	A	20030128	MX 2002-PA9382	20020925 <--
US 2003212012	A1	20031113	US 2003-239912	20030210 <--
US 7211601	B2	20070501		
HK 1054031	A1	20070504	HK 2003-106333	20030905 <--
IN 2005MN01049	A	20060519	IN 2005-MN1049	20050927 <--
PRIORITY APPLN. INFO.:			EP 2000-106034	A 20000327 <--
			WO 2001-EP3171	W 20010320
			IN 2002-MN1184	A3 20020828

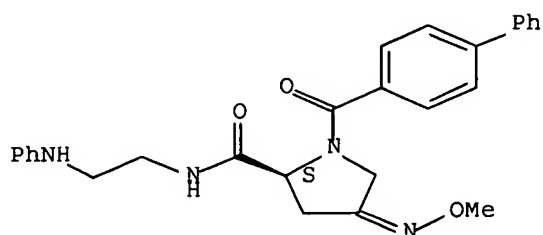
OTHER SOURCE(S):                    MARPAT 135:288686

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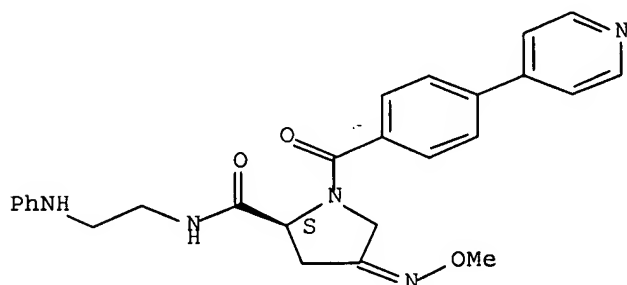
- AB Title compds. I [X = CR6R7, NOR6, NNR6R7; A = C:O, C:OO, C:NH, C:ONH, C:SNH, S:O, S:ONH, CH; B = amide or II; Q = NR10, O, S; n = 0 - 2; Y, Z, E form together with the 2 C to which they are attached a 5-6 membered (hetero)aryl; R1 = alk(en/yn)yl, (hetero)aryl, cycloalkyl, acyl, etc.; R2-5 = H, halo, alkyl, alkoxy; R6-7 = H, alk(en/yn)yl, (thio)alkoxy, halogen, CN, NO2, acyl, alkoxycarbonyl, aminocarbonyl, (hetero)cycloalkyl, etc.; R11 = H, alk(en/yn)yl, OH, SH, etc. with some provisions] were prepared and used as bax inhibitors. Over 400 compds. were disclosed. E.g., (2S)-1-(tert-butoxycarbonyl)-4-(methoxyimino)-2- pyrrolidinecarboxylic acid (preparation given) was condensed with (S)-2-amino-1-phenylethanol (THF, i-BuOCOC1, -25°C - room temperature, 16 h) and the coupled product deprotected (DCM, HCl) to give the pyrrolidine. This intermediate was condensed with 4-(2-methylphenyl)benzoic acid (DMF, ClCOCOC1, Et3N, room temperature) to give a mixture of oxime ethers which were separated by chromatog. to give III. III had IC50 = 0.07  $\mu$ M for the oxytocin receptor. I are useful in the treatment and/or prevention of disease states mediated by oxytocin, including premature labor, premature birth and dysmenorrhea.
- IC ICM C07D207-22  
ICS C07D405-12; C07D405-06; C07D405-14; C07D409-12; C07D403-14;  
C07D417-12; C07D401-12; C07D403-06; C07D403-04; A61K031-4025;  
A61K031-401; A61P025-00
- CC 27-10 (Heterocyclic Compounds (One Hetero Atom))  
Section cross-reference(s): 1, 63
- IT Parturition

Absolute stereochemistry.  
Double bond geometry unknown.



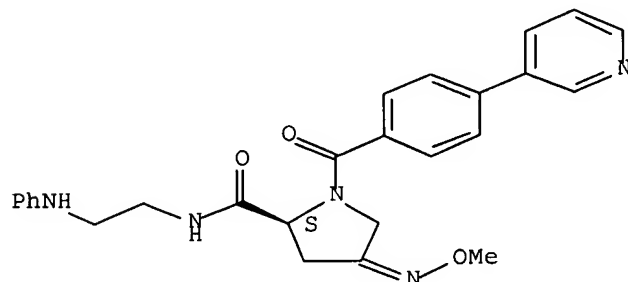
RN 365456-67-3 HCAPLUS  
CN 2-Pyrrolidinecarboxamide, 4-(methoxyimino)-N-[2-(phenylamino)ethyl]-1-[4-(4-pyridinyl)benzoyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry unknown.



RN 365456-73-1 HCAPLUS  
CN 2-Pyrrolidinecarboxamide, 4-(methoxyimino)-N-[2-(phenylamino)ethyl]-1-[4-(3-pyridinyl)benzoyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry unknown.



RN 365456-76-4 HCAPLUS  
CN 2-Pyrrolidinecarboxamide, 4-(methoxyimino)-N-[2-(phenylamino)ethyl]-1-[4-(2-pyridinyl)benzoyl]-, (2S)- (CA INDEX NAME)

SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,  
YU, ZA, ZW  
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

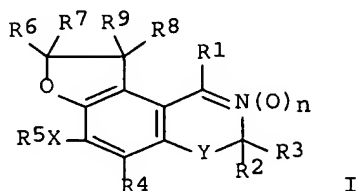
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AU 200139550	A	20011003	AU 2001-39550	20010322 <--
EP 1270577	A1	20030102	EP 2001-914191	20010322 <--
EP 1270577	B1	20061206		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

AT 347557	T	20061215	AT 2001-914191	20010322 <--
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US 2004092582	A1	20040513	US 2002-239439	20020920 <--
US 6924292	B2	20050802		

PRIORITY APPLN. INFO.: JP 2000-87121 A 20000323 <--  
WO 2001-JP2277 W 20010322

OTHER SOURCE(S): CASREACT 135:272895; MARPAT 135:272895  
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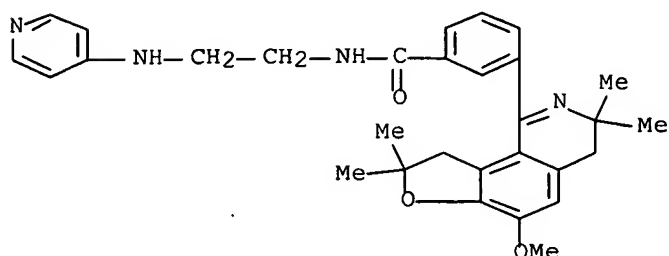


- AB Title compds. [I; R1 = C6H5, 4-HOC6H4, 1-naphthyl, 4-CH3OC6H4, 2-CH3OC6H4, 4-NH2C6H4, 4-C6H5C6H4, 4-BrC6H4, CH3, C6H5CO, 3-CH3SCH2CONHC6H4, 3-CH3OCOC6H4, 3-NH2C(CH3)2CONHC6H4, 3-furyl, 3-HOCC6H4, 2-chloro-4-pyridyl, 3-CH3CH2OCOC6H4, 4-pyridylethylaminocarbonyl; R2 = CH3, CH2Br, CH3CH2, H, CH3COO; R3 = CH3, H; R2R3 = (CH2)5; R4 = H, CH2N(CH3)2, CH2SC6H5, CH2C(:CH2)CH3, CH2NHCOCH3, CH3OCH2, CH2OH, CH2F, CH2COOH, CH2CN; R5 = Cl, OCH3, CON(CH3)2, CH3O, H, CH3CH2O, NH2, CHONH, CH3SO2NH, NH2CONH, CH3CH2S, CH3; R6 = CH3, H, CH3CH; R7 = CH3, H, CH3CH2; R6R7 = (CH2)5; R8 = H, CH3; R9 = H, CH3; Y = CH2, CHOH, C:O, C(CH3)2; X = electron pair, O, S; n = 0, 1] and salts are prepared as phosphodiesterase IV inhibitors. Title compds. are useful as preventives and remedies for diseases caused by inflammation, for example, bronchial asthma, chronic obstructive pulmonary disease (COPD), rheumatoid arthritis, autoimmune disease and diabetes. Thus, the title compound I (R6 = CH3; R7 = CH3; R2 = CH3; R3 = CH3; X = O; R5 = CH3; n = 0; R9 = H; R8 = H; R1 = 3-CH3S:OCH2CONHC6H4) was prepared and biol. tested.
- IC ICM C07D491-048  
ICS C07D453-02; C07D519-00; A61K031-4741; A61P043-00; A61P029-00; A61P011-00; A61P011-06; A61P019-02; A61P037-06; A61P003-10; C12N001-20; C12N015-00
- CC 27-17 (Heterocyclic Compounds (One Hetero Atom))  
Section cross-reference(s): 1, 63
- IT Allergy inhibitors  
Anti-inflammatory agents  
Antiarthritics  
Antiasthmatics  
Antidiabetic agents  
Antimicrobial agents

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL  
(Biological study); PREP (Preparation); USES (Uses)  
(preparation of furano-isoquinoline derivs. as phosphodiesterase IV  
inhibitors)

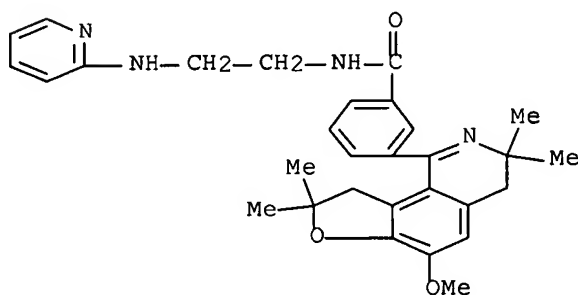
RN 362709-34-0 HCAPLUS

CN Benzamide, N-[2-(4-pyridinylamino)ethyl]-3-(3,4,8,9-tetrahydro-6-methoxy-  
3,3,8,8-tetramethylfuro[2,3-h]isoquinolin-1-yl)- (CA INDEX NAME)



RN 362709-35-1 HCAPLUS

CN Benzamide, N-[2-(2-pyridinylamino)ethyl]-3-(3,4,8,9-tetrahydro-6-methoxy-  
3,3,8,8-tetramethylfuro[2,3-h]isoquinolin-1-yl)- (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 23 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:489372 HCAPLUS Full-text

DOCUMENT NUMBER: 135:92649

TITLE: Preparation of quinazoline and quinoline derivatives  
as remedies for diseases mediated by  
autophosphorylation of PDGF receptors

INVENTOR(S): Sakai, Teruyuki; Senga, Teruhumi; Furuta, Takayuki;  
Miwa, Atushi

PATENT ASSIGNEE(S): Kirin Beer Kabushiki Kaisha, Japan

SOURCE: PCT Int. Appl., 1068 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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ICS C07D239-88; C07D401-12; C07D403-12; C07D405-12; A61K031-47;  
 A61K031-496; A61K031-5377; A61K031-505; A61K031-4709; A61K031-517;  
 A61P043-00; A61P009-10

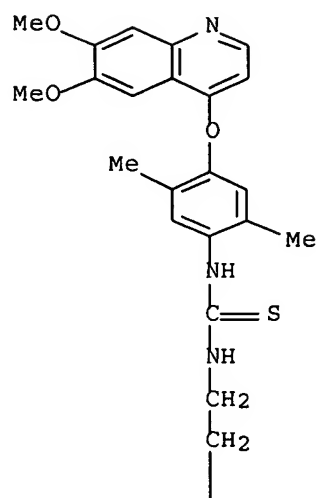
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1, 63

IT Anti-ischemic agents  
 Antirheumatic agents  
 Cirrhosis  
 Ischemia  
 Rheumatoid arthritis  
 Vasoconstriction

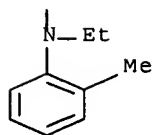
(preparation of quinazolines and quinolines as remedies for diseases  
 mediated by autophosphorylation of PDGF receptors)

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PAGE 1-A

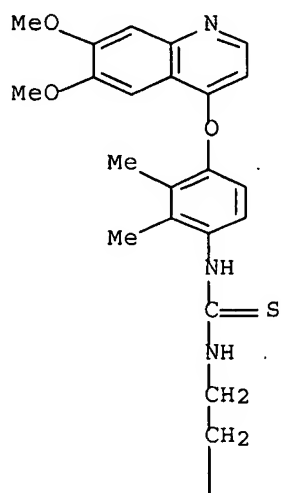


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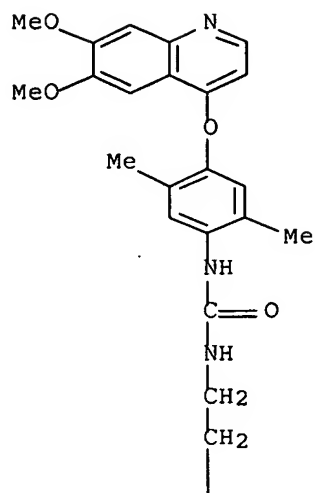


RN 347155-07-1 HCAPLUS  
 CN Thiourea, N-[4-[(6,7-dimethoxy-4-quinolinyl)oxy]-2,3-dimethylphenyl]-N'-[2-ethyl(2-methylphenyl)amino]ethyl - (CA INDEX NAME)

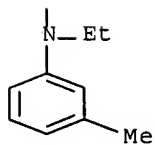
PAGE 1-A



PAGE 1-A



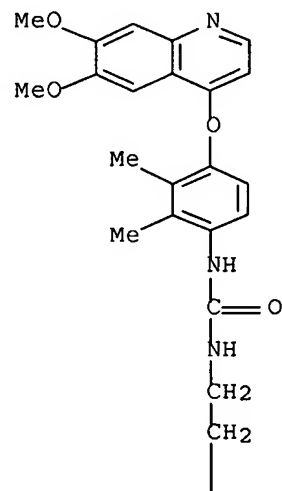
PAGE 2-A



RN 347156-23-4 HCAPLUS

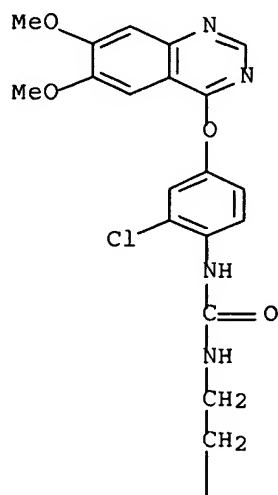
CN Urea, N-[4-[(6,7-dimethoxy-4-quinolinyl)oxy]-2,3-dimethylphenyl]-N'-[2-ethyl(3-methylphenyl)amino]ethyl]- (CA INDEX NAME)

PAGE 1-A

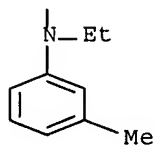




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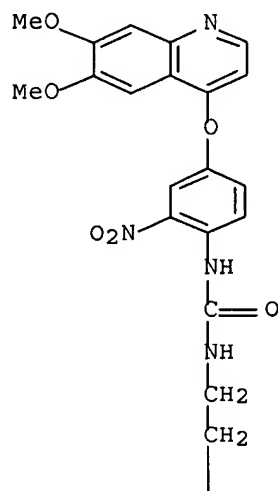


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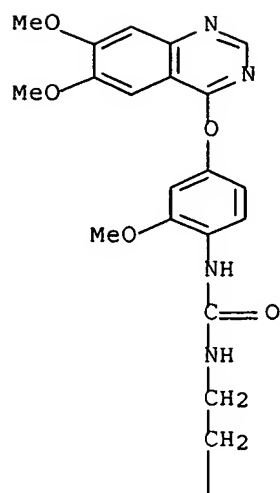


RN 347156-26-7 HCAPLUS  
 CN Urea, N-[4-[(6,7-dimethoxy-4-quinolinyl)oxy]-2-nitrophenyl]-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]- (CA INDEX NAME)

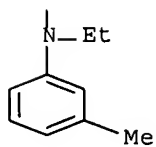
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PAGE 1-A

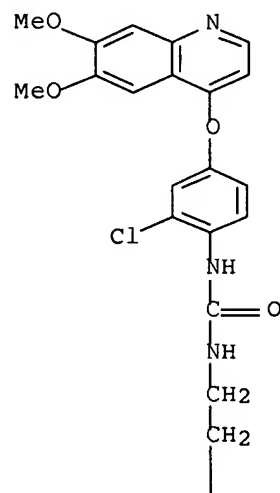


PAGE 2-A



RN 347156-29-0 HCAPLUS  
 CN Urea, N-[2-chloro-4-[(6,7-dimethoxy-4-quinolinyl)oxy]phenyl]-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]- (CA INDEX NAME)

PAGE 1-A



PATENT ASSIGNEE(S): Gabriel; Pan, Gonghua  
 SOURCE: Pharmacoepia, Inc., USA  
 PCT Int. Appl., 231 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001005783	A1	20010125	WO 2000-US19185	20000714 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2379064	A1	20010125	CA 2000-2379064	20000714 <--
EP 1196411	A1	20020417	EP 2000-950343	20000714 <--
EP 1196411	B1	20030917		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2003505384	T	20030212	JP 2001-511442	20000714 <--
AT 250053	T	20031015	AT 2000-950343	20000714 <--
AU 777735	B2	20041028	AU 2000-63459	20000714 <--
US 2003229092	A1	20031211	US 2002-46616	20020114 <--
US 6919347	B2	20050719		
HK 1048305	A1	20040723	HK 2002-107514	20021016 <--
PRIORITY APPLN. INFO.:			US 1999-143990P	P 19990715 <--
			WO 2000-US19185	W 20000714 <--
OTHER SOURCE(S):	MARPAT 134:116237			
GI				

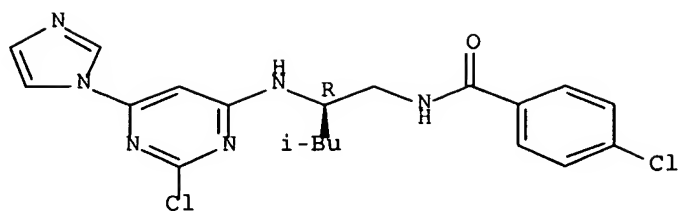
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Compds. I [X, Y, Z = CH or N; A = A1 or A2, where A1 is R4R5NCO (R4 = H, aryl, heteroaryl, substituted alkyl; R5 = H, alkyl), 5-aryl-1,2,4-triazol-3-yl, 2-aryl-4-imidazolyl, or 2-aryl-5-thiazolyl and A2 is R7CONH (R7 = aryl or alkylaryl), R7SO2NH, R4NH, R4O; Q = heteroaryl, aryl, CH2R13 (R13 = OH, OTHP, 1-imidazolyl, 1-pyrrolyl), CH:NOMe, or 1,3-dithian-2-yl; W = H, Cl, F, alkyl, aryl, heteroaryl, alkoxy, alkylthio, an amino group, arylcarbamoyl, etc.; R1 = alkyl, cycloalkyl, heterocyclyl, aryl, heteroaryl, etc.; R2 = H or alkyl or R1R2C is a ring optionally containing O, S or N; R3 = H or alkyl, or when n is zero, R2 and R3 taken together form a 6-membered ring (with provisos)] were prepared as bradykinin B1 receptor antagonists. Thus, D-leucine derivative II was prepared by substitution reaction of D-leucine 4-chlorobenzylamide with 2,4-dichloro-(or difluoro)-6-(1H-imidazol-1-yl)pyrimidine and then 3-chlorobenzylamine. Pharmaceutical formulations containing II are described.

IC ICM C07D403-04

ICS C07D403-06; C07D405-04; C07D239-48; C07D239-42; C07D401-04;  
 C07D405-14; C07D409-04; C07D417-04; C07D413-04; C07D401-14;  
 A61K031-506; A61P029-00

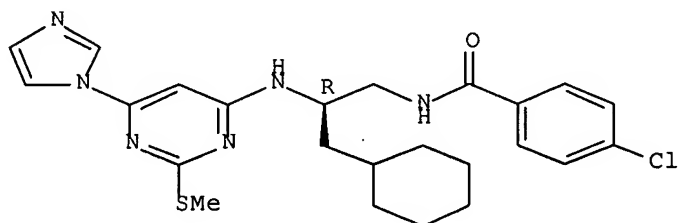
CC 34-2 (Amino Acids, Peptides, and Proteins)



RN 321329-69-5 HCAPLUS

CN Benzamide, 4-chloro-N-[(2R)-3-cyclohexyl-2-[[6-(1H-imidazol-1-yl)-2-(methylthio)-4-pyrimidinyl]amino]propyl]- (CA INDEX NAME)

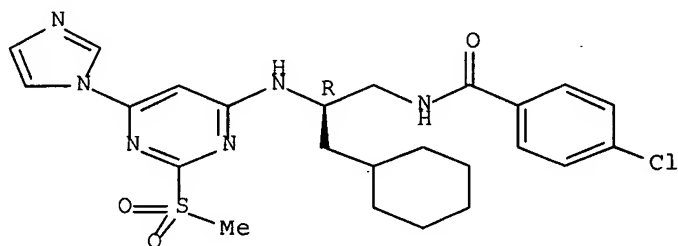
Absolute stereochemistry.



RN 321329-71-9 HCAPLUS

CN Benzamide, 4-chloro-N-[(2R)-3-cyclohexyl-2-[[6-(1H-imidazol-1-yl)-2-(methylsulfonyl)-4-pyrimidinyl]amino]propyl]- (CA INDEX NAME)

Absolute stereochemistry.



IT 321328-76-1P 321329-73-1P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of bradykinin B1 receptor antagonists)

RN 321328-76-1 HCAPLUS

CN Benzamide, 4-chloro-N-[(2R)-2-[[2-[[[3-chlorophenyl)methyl]amino]-6-(1H-imidazol-1-yl)-4-pyrimidinyl]amino]-4-methylpentyl]- (CA INDEX NAME)

Absolute stereochemistry.

CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,  
 HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,  
 LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,  
 SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,  
 YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,  
 CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2370344 A1 20010111 CA 2000-2370344 20000630 <--  
 EP 1192164 A1 20020403 EP 2000-940670 20000630 <--  
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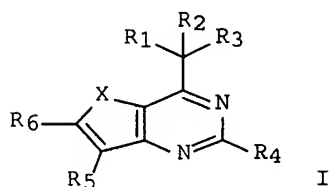
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 US 6787541 B1 20040907 US 2002-958948 20020313 <--

PRIORITY APPLN. INFO.:

GB 1999-15437 A 19990701 <--  
 WO 2000-GB2517 W 20000630 <--

OTHER SOURCE(S): MARPAT 134:100882

GI



AB Thieno- and furopyrimidines I [X = O or S; R1 and R2 are independently selected from hydrogen, alkyl, aryl, hydroxy, alkoxy, aryloxy, cyano, nitro, CO2R7, COR7, OCOR7CONR7R8, CONR7NR8R9, OCONR7R8, NR7R8, NR7COR8, NR7CONR8R9, NR7CO2R8, NR7SO2R8, NR7CONR8NR9R10, NR7NR8CO2R9, NR7NR8CONR9R10, NR7SO2NR8R9, SO2R7, SOR7, SR7 and SO2NR7R8, or R1 and R2 together form a carbonyl group (C=O), an oxime group (C=NOR11), an imine group (C=NR11) or a hydrazone group (C=NNR11R12), or R1 and R2 together form a 5, 6 or 7 membered carbocyclic or heterocyclic ring; R3 is alkyl or aryl; R4, R5 and R6 are independently selected from hydrogen, alkyl, aryl, halogen, hydroxy, nitro, cyano, alkoxy, aryloxy, COR7, OCOR7, CO2R7, SR7, SOR7, SO2R7, SO2NR7R8, CONR7R8, CONR7NR8R9, OCONR7R8, NR7R8, NR7COR8, NR7CONR8R9, NR7CO2R8, NR7SO2R8, CR7=NOR8, NR7CONR8NR9R10, NR7NR8CO2R9, NR7NR8CONR9R10, SO2NR7NR8R9, NR7SO2NR8R9, NR7NR8SO2R9, NR7NR8COR9, NR7NR8R9 and NR7CSNR8R9, or R5 and R6 together form a 5, 6 or 7 membered carbocyclic or heterocyclic ring; R7, R8, R9, R10, R11 and R12 are independently selected from hydrogen, alkyl and aryl] or a pharmaceutically acceptable salt thereof or prodrug thereof, are prepared as antagonists of purine receptors, and the use thereof in therapy, particularly in the therapy of a disorder in which the blocking of purine receptors may be beneficial, such as Parkinson's Disease and other movement disorders. In particular, I are tested for their activity as antagonists of the adenosine A2a receptor. E.g., thienopyrimidine I (X = S; R1 = R2 = O; R3 = Ph; R4 = F3C; R5 = R6 = H) (II) was prepared by treatment of a solution of 4-chloro-2-(trifluoromethyl)thieno[3,2-d]pyrimidine, benzaldehyde, and N,N-dimethylimidazolium iodide in THF with sodium hydride; the solution was then refluxed for 15 min. and cooled to room temperature to give, after workup, II in 43% yield. Biol. data on the binding of a subset of I to the adenosine A2a receptor was obtained.

IC ICM C07D495-04

(Biological study, unclassified); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

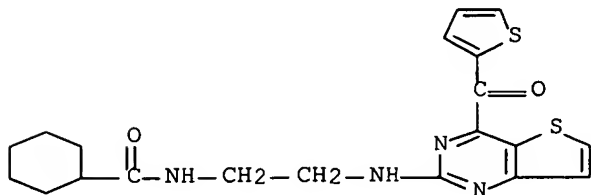
(preparation of thieno[3,2-d]pyrimidine and furo[3,2-d]pyrimidine derivs.

as

adenosine A2a receptor antagonists for the treatment of movement  
disorders such as Parkinson's disease)

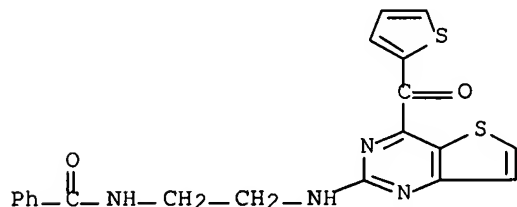
RN 319441-96-8 HCAPLUS

CN Cyclohexanecarboxamide, N-[2-[[4-(2-thienylcarbonyl)thieno[3,2-d]pyrimidin-2-yl]amino]ethyl]- (CA INDEX NAME)



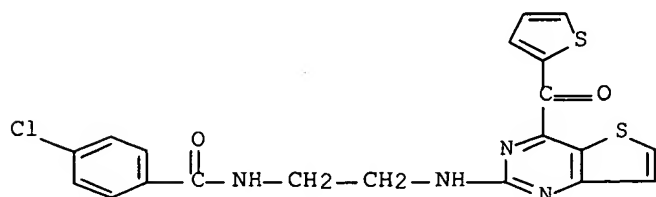
RN 319441-97-9 HCAPLUS

CN Benzamide, N-[2-[[4-(2-thienylcarbonyl)thieno[3,2-d]pyrimidin-2-yl]amino]ethyl]- (CA INDEX NAME)



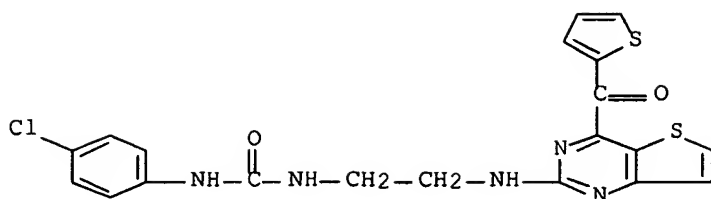
RN 319441-98-0 HCAPLUS

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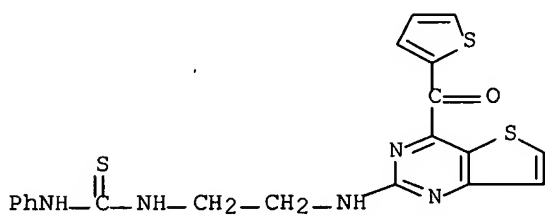
RN 319441-99-1 HCAPLUS

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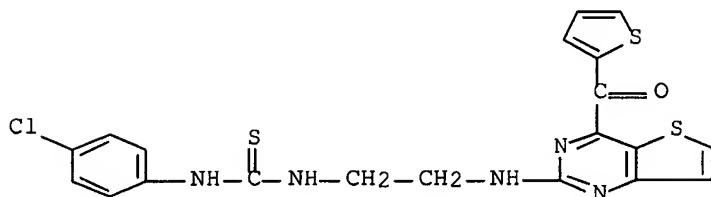
RN 319442-09-6 HCAPLUS

CN Thiourea, N-phenyl-N'-[2-[[4-(2-thienylcarbonyl)thieno[3,2-d]pyrimidin-2-yl]amino]ethyl]- (CA INDEX NAME)



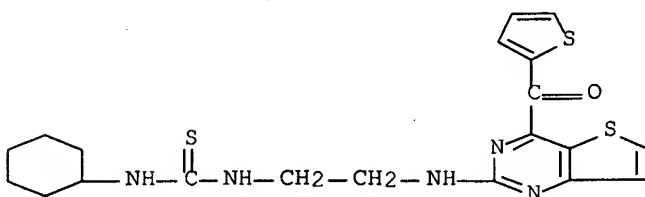
RN 319442-10-9 HCAPLUS

CN Thiourea, N-(4-chlorophenyl)-N'-[2-[[4-(2-thienylcarbonyl)thieno[3,2-d]pyrimidin-2-yl]amino]ethyl]- (CA INDEX NAME)



RN 319442-11-0 HCAPLUS

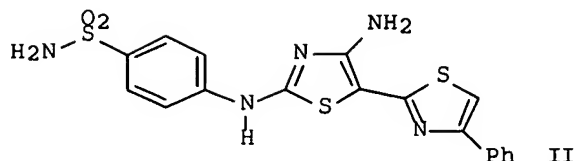
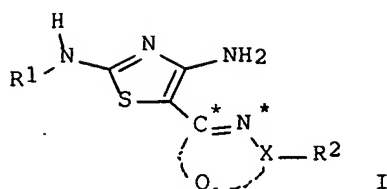
CN Thiourea, N-cyclohexyl-N'-[2-[[4-(2-thienylcarbonyl)thieno[3,2-d]pyrimidin-2-yl]amino]ethyl]- (CA INDEX NAME)



REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS



- AB The title compds. [I; R1 = H, (un)substituted alkyl, cycloalkyl, etc.; R2 = OH, halo, CN, etc.; X = C, N; Q = a divalent radical having 2 or 3 atoms selected from C, N, O, S, CR5, NR5 (wherein R5 = OH, halo, CN, etc.) which together with C\* and N\* form a 5-6 membered (non)aromatic ring] which modulate and/or inhibit the activity of certain protein kinases (biol. data were given), and are useful in treating cancer as well as other disease states associated with unwanted angiogenesis and/or cellular proliferation, such as diabetic retinopathy, neovascular glaucoma, rheumatoid arthritis, and psoriasis, were prepared and formulated. E.g., a multi-step synthesis of diaminothiazole II was given. The compds. I and pharmaceutical compns. containing them are capable of mediating tyrosine kinase signal transduction in order to modulate and/or inhibit unwanted cell proliferation.
- IC ICM C07D277-38  
ICS C07D277-62; C07D417-04; C07D417-14; C07F009-6539; A61K031-426; A61K031-427; A61P035-00
- CC 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1, 63
- ST aminothiazole prepn protein kinase inhibition; thiazole amino prepn protein kinase inhibition; vascular endothelial growth factor receptor aminothiazole prepn; VEGF receptor aminothiazole prepn; fibroblast growth factor receptor aminothiazole prepn; FGF receptor aminothiazole prepn; tyrosine kinase LCK aminothiazole prepn; cyclin complex cdk protein kinase aminothiazole prepn; animal cell line HUVEC proliferation inhibition aminothiazole prepn; antitumor aminothiazole prepn; angiogenesis aminothiazole prepn; diabetic retinopathy aminothiazole prepn; glaucoma neovascular aminothiazole prepn; rheumatoid arthritis aminothiazole prepn; psoriasis aminothiazole prepn
- IT Antitumor agents  
Combinatorial library  
Proliferation inhibition  
Psoriasis  
Rheumatoid arthritis  
(preparation of diaminothiazoles for inhibiting protein kinases)
- IT
- |             |             |             |             |             |
|-------------|-------------|-------------|-------------|-------------|
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RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); THU (Therapeutic use); BIOL  
 (Biological study); USES (Uses)

(preparation of diaminothiazoles for inhibiting protein kinases)

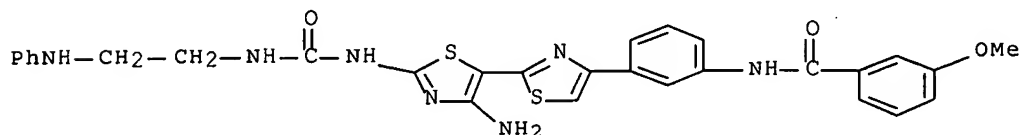
IT 312766-80-6 312767-67-2 312767-77-4  
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RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); THU (Therapeutic use); BIOL  
 (Biological study); USES (Uses)

(preparation of diaminothiazoles for inhibiting protein kinases)

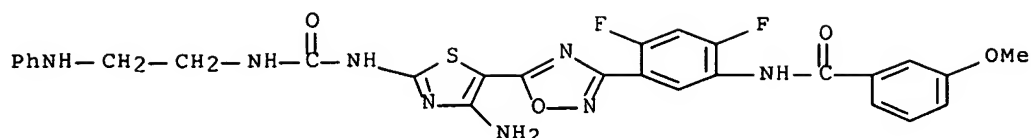
RN 312766-80-6 HCAPLUS

CN Benzamide, N-[3-[4'-amino-2'-[[[2-(phenylamino)ethyl]amino]carbonyl]amino  
 ] [2,5'-bithiazol]-4-yl]phenyl]-3-methoxy- (CA INDEX NAME)



RN 312767-67-2 HCAPLUS

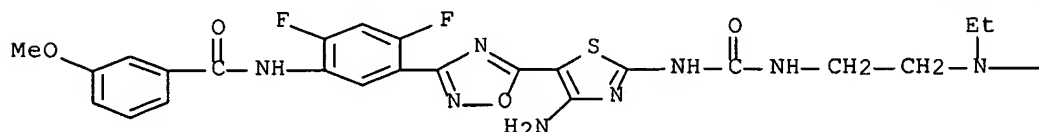
CN Benzamide, N-[3-[4'-amino-2'-[[[2-[ethyl(3-methylphenyl)amino]ethyl]amino]  
 ]carbonyl]amino] [2,5'-bithiazol]-4-yl]phenyl]-3-methoxy- (CA INDEX NAME)



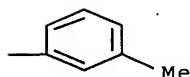
RN 312769-21-4 HCAPLUS

CN Benzamide, N-[5-[5-[4-amino-2-[[[2-[ethyl(3-methylphenyl)amino]ethyl]amino]carbonyl]amino]-5-thiazolyl]-1,2,4-oxadiazol-3-yl]-2,4-difluorophenyl]-3-methoxy- (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 27 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:421119 HCAPLUS Full-text

DOCUMENT NUMBER: 133:58807

TITLE: Preparation of morpholine derivatives as selective antagonists of  $\alpha_1$  receptors.

INVENTOR(S): Lagu, Bharat; Nagarathnam, Dhanapalan; Tian, Dake; Gluchowski, Charles

PATENT ASSIGNEE(S): Synaptic Pharmaceutical Corporation, USA

SOURCE: PCT Int. Appl., 132 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000035891	A1	20000622	WO 1999-US30259	19991217 <--
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,				

277295-78-0P 277295-79-1P 277295-80-4P 277295-81-5P 277295-82-6P  
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RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(preparation of morpholine derivs. as selective antagonists of  $\alpha_1$   
 receptors)

IT 277295-75-7P 277295-84-8P 277295-88-2P

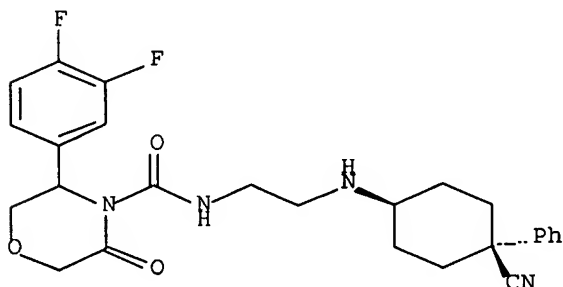
RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(preparation of morpholine derivs. as selective antagonists of  $\alpha_1$   
 receptors)

RN 277295-75-7 HCAPLUS

CN 4-Morpholinecarboxamide, N-[2-[(cis-4-cyano-4-  
 phenylcyclohexyl)amino]ethyl]-3-(3,4-difluorophenyl)-5-oxo-,  
 monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.

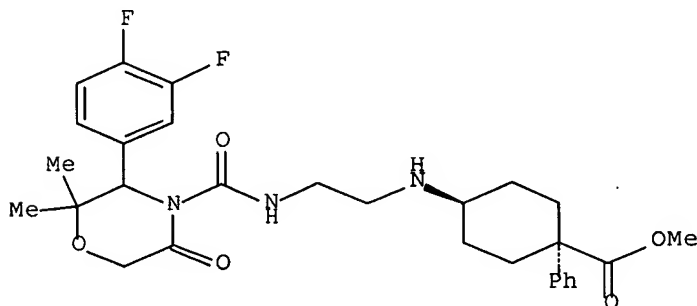


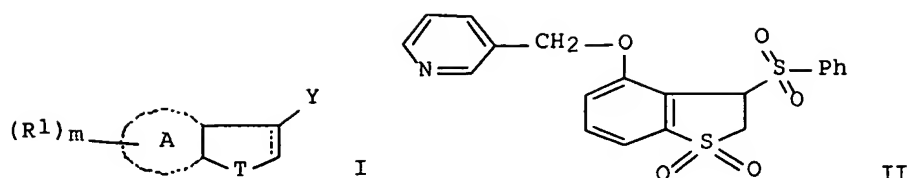
● HCl

RN 277295-84-8 HCAPLUS

CN Cyclohexanecarboxylic acid, 4-[[2-[[[3-(3,4-difluorophenyl)-2,2-dimethyl-5-  
 oxo-4-morpholinyl]carbonyl]amino]ethyl]amino]-1-phenyl-, methyl ester,  
 cis- (CA INDEX NAME)

Relative stereochemistry.





AB The title compds. I [dotted line indicates single or double bond; T = S(O) $n$ ; Y = H, etc.; ring A = benzene ring, etc.; R $^1$  = alkyl, nitro, etc.; m = 0, or 1 - 4; n = 0 or 1 or 2] are prepared. The fused thiophene derivs. represented by general formula I are useful as preventives and/or remedies for various inflammatory diseases, sepsis, multiple myeloma, plasma cell leukemia, osteoporosis, cachexia, psoriasis, nephritis, renal cell cancer, Kaposi's sarcoma, chronic rheumatoid arthritis, hypergammaglobulinemia, Curschmann's disease, intraatrial myxoma, diabetes, autoimmune diseases, hepatitis, multiple sclerosis, colon inflammation, graft-vs.-host disease and infectious diseases. Formulations containing I are given. In an in vitro test using cells, the title compound II showed IC $_{50}$  of 4.4  $\mu$ M against interleukin-6 production.

IC ICM C07D333-62

ICS C07D333-54; C07D409-12; C07D409-14; C07D495-04; A61K031-38;

A61K031-40; A61K031-44; A61K031-445; A61K031-495; A61K031-535

CC 27-9 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1, 28, 63

IT Autoimmune disease

Cachexia

Diabetes mellitus

Hepatitis

Infection

Multiple myeloma

Multiple sclerosis

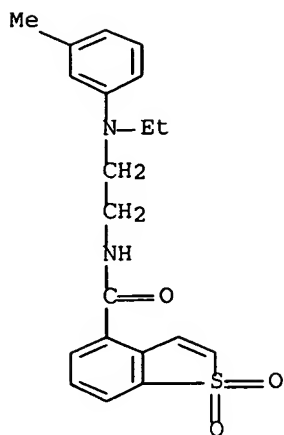
Osteoporosis

Psoriasis

Rheumatoid arthritis

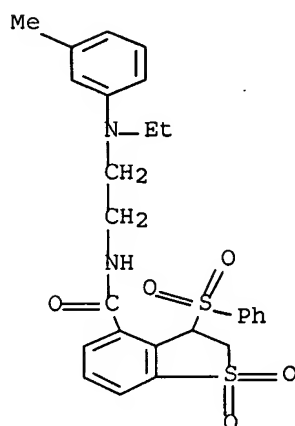
(preparation and effect of fused thiophene derivs. with activity against interleukin-6 and interleukin-12 production)

IT	246173-69-3P	246173-70-6P	246173-71-7P	246173-72-8P	246173-73-9P
	246173-74-0P	246173-75-1P	246173-77-3P	246173-78-4P	246173-79-5P
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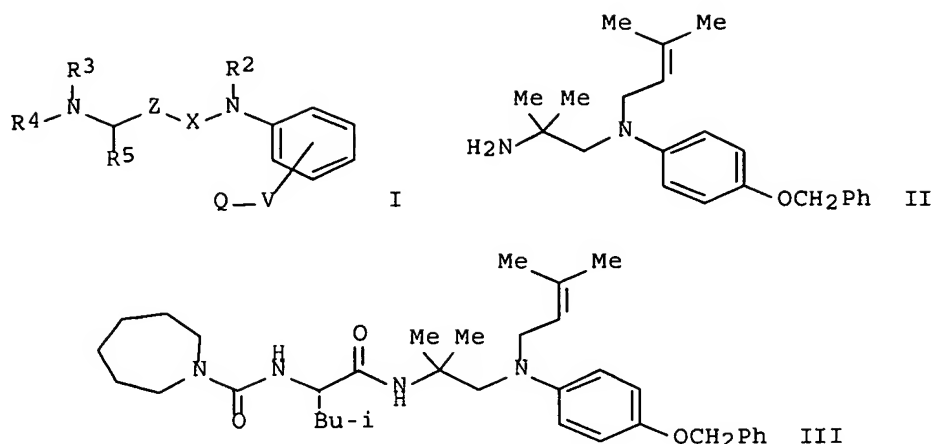
RN 246175-83-7 HCAPLUS

CN Benzo[b]thiophene-4-carboxamide, N-[2-[ethyl(3-methylphenyl)amino]ethyl]-2,3-dihydro-3-(phenylsulfonyl)-, 1,1-dioxide (CA INDEX NAME)



RN 246175-84-8 HCAPLUS

CN Benzo[b]thiophene-4-carboxamide, N-[2-[ethyl(3-methylphenyl)amino]ethyl]-2,3-dihydro-3-(phenylsulfonyl)-, 1,1-dioxide, monohydrochloride (9CI) (CA INDEX NAME)



AB The invention provides compds. that block calcium channels. In particular, the invention claims compds. I [Z = CH<sub>2</sub> or CO; X = cycloalkylene, (un)substituted heterocycloalkylene, imino or iminoalkylene, certain piperidinediyl or pyrrolidinediyl radicals or their alkylene derivs.; Q = H, (un)substituted aryl, heteroaryl, cycloalkyl, alkyl, heterocycloalkyl; V = O(CH<sub>2</sub>)<sub>n</sub> or (CH<sub>2</sub>)<sub>n</sub>O, O, (CH<sub>2</sub>)<sub>n</sub>, CH:CH, NH(CH<sub>2</sub>)<sub>n</sub> or (CH<sub>2</sub>)<sub>n</sub>NH or derivs.; R<sub>2</sub> = H, alkenyl, cycloalkenyl, (un)substituted Ph, alkyl, cycloalkyl, or Ph; R<sub>3</sub> = H, alkyl, alkenyl; R<sub>4</sub> = H, cyclo-(CH<sub>2</sub>)<sub>m</sub>NCO, alkyl, alkenyl, (un)substituted Ph, heteroaryl, or cycloalkyl; or NR<sub>3</sub>R<sub>4</sub> = 5- to 7-membered ring with an optional addnl. heteroatom; R<sub>5</sub> = alkyl, (un)substituted Ph or heteroaryl; m = 1-3; n = 0-3] and their pharmaceutically acceptable salts, esters, amides, and prodrugs. The invention also provides methods of using the compds. to treat stroke, cerebral ischemia, head trauma, or epilepsy, and to pharmaceutical compns. that contain the compds. Over 50 synthetic examples are given, and these plus a large number of addnl. invention compds. are specifically claimed. For instance, N-BOC-α-aminoisobutyric acid underwent amidation with 4-benzyloxylaniline, followed by reduction of the amide with diborane, N-alkenylation with 4-bromo-2-methyl-2-butene, and acidic deprotection to remove BOC, to give intermediate II. In a sep. preparation, H-Leu-OCH<sub>2</sub>Ph was treated with triphosgene and hexamethylenamine, then deprotected, to give Hac-Leu-OH (III; Hac = hexamethylenaminocarbonyl). Coupling of II with III using HBTU and DIPEA in DMF gave title compound IV. The latter blocked calcium flux through N-type Ca<sup>2+</sup> channels in IMR-32 neuronal tumor cells in vitro, with IC<sub>50</sub> of 0.26 μM. Selected compds. gave 20-100% protection of mice from tonic seizures in a sound chamber, at doses of 10-30 mg/kg i.v.

IC ICM C07D295-20

ICS A61K031-55; C07D211-58; C07C233-36; A61K031-16; C07D401-12;  
A61K031-445

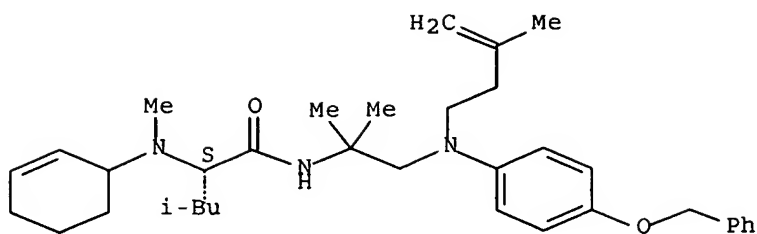
CC 27-21 (Heterocyclic Compounds (One Hetero Atom))  
Section cross-reference(s): 1, 25

IT Analgesics

Anticonvulsants

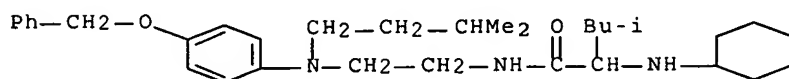
(preparation of aniline derivs. as calcium channel blockers)

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	220737-41-7P	220737-42-8P	220737-43-9P	220737-44-0P	220737-45-1P
	220737-46-2P	220737-47-3P	220737-48-4P	220737-49-5P	
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	220737-57-5P	220737-58-6P	220737-59-7P	220737-60-0P	220737-61-1P



RN 220738-18-1 HCAPLUS

CN Pentanamide, 2-(cyclohexylamino)-4-methyl-N-[2-[(3-methylbutyl)[4-(phenylmethoxy)phenyl]amino]ethyl]- (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 30 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:816104 HCAPLUS Full-text

DOCUMENT NUMBER: 130:66484

TITLE: Preparation of isoxazoline and isoxazole fibrinogen receptor antagonists

INVENTOR(S): Wityak, John; Xue, Chu-Biao; Sielecki-Dzurdz, Thais Motria; Olson, Richard Eric; Degrado, William Frank; Cain, Gary Avonn; Batt, Douglas Guy; Pinto, Donald; Hussain, Munir Alwan; Mousa, Shaker Ahmed

PATENT ASSIGNEE(S): The DuPont Merck Pharmaceutical Company, USA

SOURCE: U.S., 153 pp., Cont.-in-part of U.S. Ser. No. 337,920, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5849736	A	19981215	US 1995-455436	19950531 <--
CA 2174838	A1	19950601	CA 1994-2174838	19941114 <--
HU 74690	A2	19970128	HU 1996-1414	19941114 <--
EP 970950	A2	20000112	EP 1999-119541	19941114 <--
EP 970950	A3	20000405		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
ES 2154326	T3	20010401	ES 1995-901915	19941114 <--
PT 730590	T	20010531	PT 1995-901915	19941114 <--
IL 111721	A	20000601	IL 1994-111721	19941121 <--
TW 483895	B	20020421	TW 1994-83110865	19941122 <--
ZA 9409337	A	19960524	ZA 1994-9337	19941124 <--
IL 118262	A	20030212	IL 1996-118262	19960515 <--
CA 2222147	A1	19961205	CA 1996-2222147	19960530 <--
WO 9638426	A1	19961205	WO 1996-US7692	19960530 <--

restenosis, atherosclerosis, stroke, myocardial infarction, and unstable angina. In particular, title compds. I are claimed [wherein: R1 = a variety of cyclic and/or acyclic N-containing groups; R2 = H, alk(en/yn)yl, alkoxy, aryl, heteroaryl, CO<sub>2</sub>H or certain derivs.; R3 = H, OH, alky(en/yn)yl, alkoxy, alkoxycarbonyl, (un)substituted aryl or heterocyclyl, etc.; U = single bond, alk(en/yn)ylene; V = single bond, (un)substituted alk(en/yn)ylene, C<sub>6</sub>H<sub>4</sub>, pyridinediyl, pyridazinediyl; W = (un)substituted (CH<sub>2</sub>)<sub>n</sub>CONH or CONH(CH<sub>2</sub>)<sub>n</sub>; X = (un)substituted alkylene; Y = OH and derivs.]. For instance, 4-hydroxybenzaldehyde was etherified with 2-[N-(tert-butoxycarbonyl)piperidin-4-yl]ethanol by Mitsunobu reaction (70%), followed by oximation of the aldehyde with NH<sub>2</sub>OH (87%), chlorination of the oxime to give an oximinoyl chloride (52%), dipolar cycloaddn. of this with Me 3-butenate (77%), saponification of the Me ester (74%), and hydrolysis of the BOC group with CF<sub>3</sub>CO<sub>2</sub>H (TFA), to give title compound II.TFA in 60% yield. II inhibited aggregation of human platelets in vitro, using a variety of agonists, with IC<sub>50</sub> of < 10 μM.

IC ICM C07D261-02

ICS C07D217-00; A61K031-54; A61K031-445

INCL 514227800

CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 63

ST fibrinogen receptor antagonist isoxazoline isoxazole prepn; antithrombotic isoxazoline isoxazole prepn; platelet aggregation inhibitor isoxazoline isoxazole prepn; restenosis inhibitor isoxazoline isoxazole prepn; antiatherosclerotic isoxazoline isoxazole prepn; stroke treatment isoxazoline isoxazole prepn; myocardial infarction treatment isoxazoline isoxazole prepn; angina treatment isoxazoline isoxazole prepn; rheumatoid arthritis treatment isoxazoline isoxazole prepn; antiasthmatic isoxazoline isoxazole prepn; allergy inhibitor isoxazoline isoxazole prepn; organ transplantation rejection isoxazoline isoxazole prepn; septic shock isoxazoline isoxazole prepn; psoriasis isoxazoline isoxazole prepn; contact dermatitis isoxazoline isoxazole prepn; osteoporosis treatment isoxazoline isoxazole prepn; osteoarthritis treatment isoxazoline isoxazole prepn; tumor metastasis treatment isoxazoline isoxazole prepn; diabetic retinopathy treatment isoxazoline isoxazole prepn; antiinflammatory isoxazoline isoxazole prepn

IT Osteoarthritis

Osteoporosis

Psoriasis

Rheumatoid arthritis

Thrombosis

(treatment; preparation of novel isoxazoline and isoxazole fibrinogen receptor antagonists)

IT	170229-10-4P	170722-86-8P	170722-89-1P	170722-99-3P	170723-02-1P
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 186051-60-5P 186051-61-6P

RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(preparation of novel isoxazoline and isoxazole fibrinogen receptor  
 antagonists)

IT 170724-02-4P 185967-17-3P

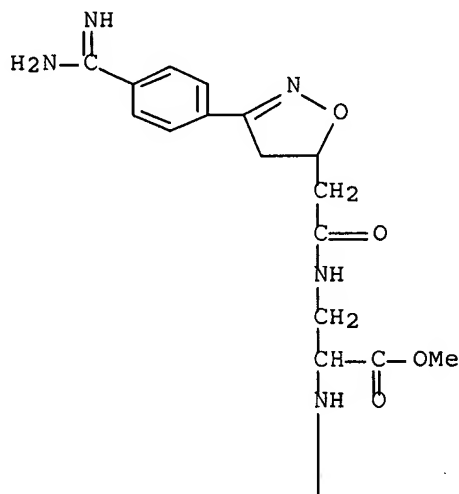
RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(preparation of novel isoxazoline and isoxazole fibrinogen receptor  
 antagonists)

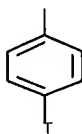
RN 170724-02-4 HCAPLUS

CN Alanine, 3-[[[3-[4-(aminoiminomethyl)phenyl]-4,5-dihydro-5-  
 isoxazolyl]acetyl]amino]-N-(4-iodophenyl)-, methyl ester (9CI) (CA INDEX  
 NAME)

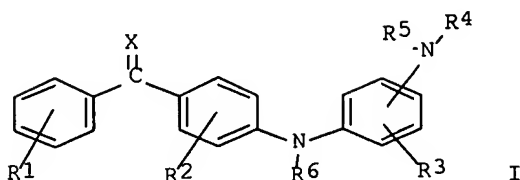
PAGE 1-A



PAGE 2-A



PT 966424	T	20040930	PT 1998-900270	19980108 <--
ES 2223116	T3	20050216	ES 1998-900270	19980108 <--
RO 120195	B1	20051028	RO 1999-839	19980108 <--
US 6313174	B1	20011106	US 1999-341923	19990721 <--
HK 1025306	A1	20050630	HK 2000-104495	20000721 <--
PRIORITY APPLN. INFO.:			GB 1997-1453	A 19970124 <--
			WO 1998-DK8	W 19980108 <--
OTHER SOURCE(S):		MARPAT 129:148822		
GI				



AB The title compds. I [R1 and R2 stand independently for one or more, similar or different substituents selected from the group consisting of hydrogen, halogen, hydroxy, mercapto, trifluoromethyl, amino, alkyl, alkoxy, alkylthio, alkylamino, or alkoxycarbonyl, the C-content of which can be from 1 to 5, cyano, carboxy, carbamoyl, Ph, or nitro; R3 stands for hydrogen, halogen, hydroxy, mercapto, trifluoromethyl, amino, alkyl, alkoxy, alkylthio, alkylamino, or alkoxycarbonyl, the C-content of which can be from 1 to 5, Ph, cyano, carboxy, or carbamoyl; R4, R5 and R6 stand independently for hydrogen, trifluoromethyl, alkyl, carbamoyl, alkoxycarbonyl, or alkyloxy, the C-content of which can be from 1 to 5; X stands for oxygen, NOH, NO-alkyl, dialkoxy, cyclic dialkoxy, dialkylthio, or cyclic dialkylthio, the C-content of which can be from 1 to 5] are prepared. The present compds. are of value in the human and veterinary practice as systemic and topical therapeutic agents for the treatment and prophylaxis of asthma, allergy, rheumatoid arthritis, spondyloarthritis, gout, atherosclerosis, chronic inflammatory bowel disease, proliferative and inflammatory skin disorders, such as psoriasis, and atopic dermatitis. In an in vitro test using human polymorphonuclear granulocytes, 4-(2-aminophenylamino)-2-chloro-2'-methylbenzophenone in vitro showed IC<sub>50</sub> of 13 nM and 7.1 nM against the production of IL-1 $\beta$  and TNF- $\alpha$ , resp. In the above test, 4-(2-aminophenylamino)benzophenone (II) in vitro showed IC<sub>50</sub> of 250 nM and 790 nM against the production of IL-1 $\beta$  and TNF- $\alpha$ , resp. In the 12-O-tetradecanoylphorbol-13-acetate induced murine skin inflammation model, II showed activity equal to hydrocortisone.

IC ICM C07C225-22

ICS A61K031-135

CC 25-16 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
Section cross-reference(s): 1, 63

IT Arthritis

(preparation and effect of aminobenzophenones)

IT Allergy inhibitors

Anti-inflammatory agents

Antiasthmatics

Gout

Psoriasis

Rheumatoid arthritis

(preparation and effect of aminobenzophenones as inhibitors of interleukin and TNF)

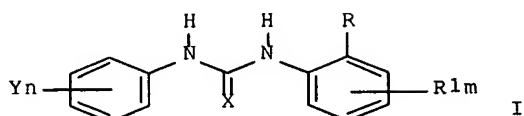
IT 210965-65-4P 210965-66-5P 210965-67-6P 210965-68-7P 210965-69-8P

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5780483	A	19980714	US 1996-701299	19960821 <--
US 5886044	A	19990323	US 1996-641990	19960320 <--
US 6211373	B1	20010403	US 1998-111663	19980708 <--
PRIORITY APPLN. INFO.:			US 1995-390260	B2 19950217 <--
			US 1996-641990	A2 19960320 <--
			WO 1996-US2260	W 19960216 <--
			US 1996-701299	A3 19960821 <--

OTHER SOURCE(S): MARPAT 129:122458

GI



AB The title compds. [I; X = O, S; R = any functional moiety having an ionizable H and a pKa of  $\leq 10$  (sic); R1, Y = H, halo, NO<sub>2</sub>, cyano, (halo)alkyl, alkenyl, (halo)alkoxy, N<sub>3</sub>, HO, hydroxyalkyl, aryl, arylalkyl, aryloxy, arylalkoxy, heteroaryl, heteroarylalkyl, heterocyclyl, heterocyclalkyl, heterocyclalkoxy, arylalkenyl, heteroarylalkenyl, (un)substituted NH<sub>2</sub>, CONH<sub>2</sub>, or SO<sub>3</sub>H, etc.; m, n = 1-3], which are useful for the treatment of disease states mediated by the chemokine, interleukin-8 (IL-8) (no data), are prepared. Thus, Me 4-amino-3- hydroxybenzoate was added to a solution of Ph isocyanate in PhMe and the resulting mixture was stirred at .apprx.80° for 24-48 h to give 90% N-[2-hydroxy-4-(methoxycarbonyl)phenyl]-N'-phenylurea.

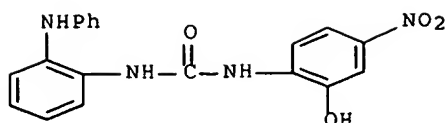
IC ICM A61K031-47  
ICS A61K031-425; A61K031-38; A61K031-17

INCL 514311000

CC 25-21 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
Section cross-reference(s): 1

ST phenylurea prepn interleukin 8 receptor antagonist; psoriasis treatment  
diphenylurea prepn; atopic dermatitis treatment diphenylurea; asthma  
treatment diphenylurea; chronic obstructive pulmonary disease treatment  
diphenylurea; adult respiratory distress syndrome treatment diphenylurea;  
arthritis treatment diphenylurea; inflammatory bowel disease  
treatment diphenylurea; Crohn disease treatment diphenylurea; ulcerative  
colitis treatment diphenylurea; septic shock treatment diphenylurea;  
endotoxic shock treatment diphenylurea; gram neg sepsis treatment  
diphenylurea; toxic shock syndrome treatment diphenylurea; cardiac renal  
reperfusion injury treatment diphenylurea; glomeruli nephritis treatment  
diphenylurea; thrombosis treatment diphenylurea; Alzheimer disease  
treatment diphenylurea; graft vs host reaction treatment diphenylurea;  
allograft rejection treatment diphenylurea; stroke treatment diphenylurea

IT 25751-87-5P 85915-46-4P 88846-90-6P 92949-89-8P 117745-32-1P  
119838-01-6P 160383-78-8P 160383-79-9P 160383-90-4P 182497-99-0P  
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REFERENCE COUNT: 84 THERE ARE 84 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 33 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1997:105201 HCAPLUS Full-text  
 DOCUMENT NUMBER: 126:117965  
 TITLE: Preparation of novel isoxazoline and isoxazole fibrinogen receptor antagonists  
 INVENTOR(S): Wityak, John; Cain, Gary Avonn; Batt, Douglas Guy; Pinto, Donald; Hussain, Munir Alwan; Xue, Chu-Biao; Sielecki-Dzurdz, Thais Motria; Olson, Richard Eric; Degrado, William Frank; Mousa, Shaker Ahmed  
 PATENT ASSIGNEE(S): Du Pont Merck Pharmaceutical Company, USA  
 SOURCE: PCT Int. Appl., 412 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9638426	A1	19961205	WO 1996-US7692	19960530 <--
W: AM, AT, AU, AZ, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, HU, JP, KG, KR, KZ, LT, LU, LV, MD, MX, NO, NZ, PL, PT, RO, RU, SE, SG, SI, SK, TJ, TM, UA, VN				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 5849736	A	19981215	US 1995-455436	19950531 <--
AU 9660243	A	19961218	AU 1996-60243	19960530 <--
AU 723577	B2	20000831		
EP 832076	A1	19980401	EP 1996-917833	19960530 <--
EP 832076	B1	20030716		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 11504651	T	19990427	JP 1996-536579	19960530 <--
BR 9609151	A	19990629	BR 1996-9151	19960530 <--
AT 245150	T	20030815	AT 1996-917833	19960530 <--
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			US 1993-157598	B2 19931124 <--
			US 1994-232961	B2 19940422 <--
			US 1994-337920	B2 19941110 <--
			WO 1996-US7692	W 19960530 <--

OTHER SOURCE(S): MARPAT 126:117965  
 GI

Rheumatoid arthritis

Thrombosis

(treatment; preparation of novel isoxazoline and isoxazole fibrinogen receptor antagonists)

IT	170229-10-4P	170722-86-8P	170722-89-1P	170722-99-3P	170723-02-1P
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RL: BAC (Biological activity or effector, except adverse); BSU

(Biological study, unclassified); SPN (Synthetic preparation); THU

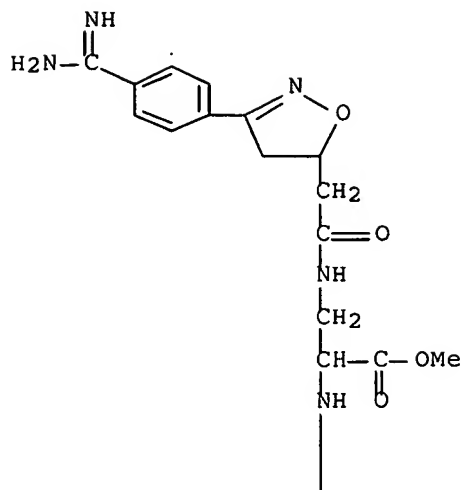
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)

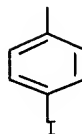
(preparation of novel isoxazoline and isoxazole fibrinogen receptor antagonists)

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	185966-88-5P	185966-90-9P	185966-92-1P	185966-93-2P	185966-95-4P
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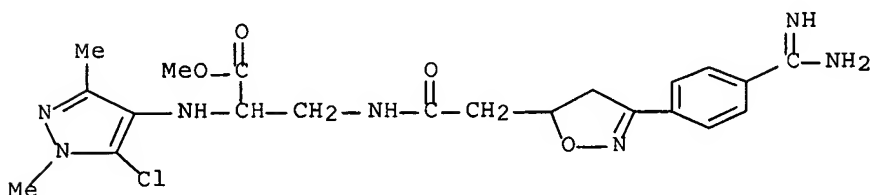
PAGE 1-A



PAGE 2-A



RN 185967-17-3 HCAPLUS  
 CN Alanine, 3-[[[3-[4-(aminoiminomethyl)phenyl]-4,5-dihydro-5-isoxazolyl]acetyl]amino]-N-(5-chloro-1,3-dimethyl-1H-pyrazol-4-yl)-, methyl ester (9CI) (CA INDEX NAME)



L163 ANSWER 34 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1997:34215 HCAPLUS Full-text  
 DOCUMENT NUMBER: 126:59946  
 TITLE: Preparation of aminothiazole derivatives as ameliorating agents for digestive tract movements  
 INVENTOR(S): Nagasawa, Masaaki; Murata, Masakazu; Nishioka, Hiroyasu; Kurimoto, Tadashi; Ueki, Shigeru; Kitagawa, Osamu  
 PATENT ASSIGNEE(S): Zeria Pharmaceutical Co., Ltd., Japan  
 SOURCE: PCT Int. Appl., 101 pp.

digestive tract movements)

IT 185103-62-2P 185103-63-3P 185103-64-4P 185103-66-6P 185103-67-7P  
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 185106-10-9P 185106-13-2P 185106-15-4P 185106-16-5P

RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(preparation of aminothiazole derivs. as ameliorating agents for digestive tract movements)

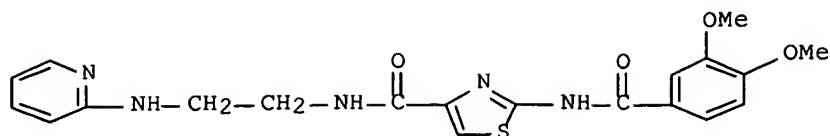
IT 185103-98-4P 185103-99-5P 185104-00-1P  
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 185105-41-3P

RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(preparation of aminothiazole derivs. as ameliorating agents for digestive tract movements)

RN 185103-98-4 HCAPLUS

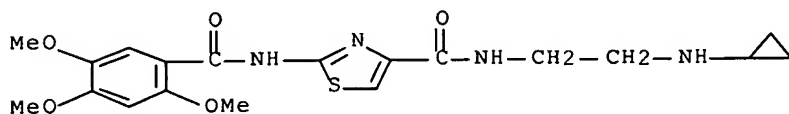
CN 4-Thiazolecarboxamide, N-[2-[(4,5-dihydro-2-thiazolyl)amino]ethyl]-2-[(3,4-dimethoxybenzoyl)amino]- (CA INDEX NAME)



● HCl

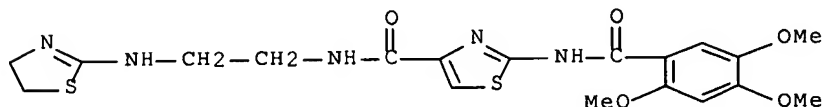
RN 185104-66-9 HCAPLUS

CN 4-Thiazolecarboxamide, N-[2-(cyclopropylamino)ethyl]-2-[(2,4,5-trimethoxybenzoyl)amino]- (CA INDEX NAME)



RN 185105-41-3 HCAPLUS

CN 4-Thiazolecarboxamide, N-[2-[(4,5-dihydro-2-thiazolyl)amino]ethyl]-2-[(2,4,5-trimethoxybenzoyl)amino]- (CA INDEX NAME)



L163 ANSWER 35 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:643902 HCAPLUS Full-text

DOCUMENT NUMBER: 125:275430

TITLE: Preparation of N,N'-diphenylurea derivatives as interleukin-8 receptor antagonists

INVENTOR(S): Widdowson, Katherine Louisa; Veber, Daniel Frank; Jurewicz, Anthony Joseph; Rutledge, Melvin Clarence, Jr.; Hertzberg, Robert Philip

PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA

SOURCE: PCT Int. Appl., 116 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 5

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9625157	A1	19960822	WO 1996-US2260	19960216 <--
W: JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 809492	A1	19971203	EP 1996-906547	19960216 <--
R: BE, CH, DE, DK, FR, GB, IT, LI, NL				
JP 11503110	T	19990323	JP 1996-525199	19960216 <--



CC 25-21 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 Section cross-reference(s): 1

ST phenylurea prepn interleukin 8 receptor antagonist; psoriasis treatment  
 diphenylurea; atopic dermatitis treatment diphenylurea; asthma treatment  
 diphenylurea; chronic obstructive pulmonary disease treatment  
 diphenylurea; adult respiratory distress syndrome treatment diphenylurea;  
 arthritis treatment diphenylurea; inflammatory bowel disease  
 treatment diphenylurea; Crohn disease treatment diphenylurea; ulcerative  
 colitis treatment diphenylurea; septic shock treatment diphenylurea;  
 endotoxic shock treatment diphenylurea; gram neg sepsis treatment  
 diphenylurea; toxic shock syndrome treatment diphenylurea; cardiac renal  
 reperfusion injury treatment diphenylurea; glomerulo nephritis treatment  
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 allograft rejection treatment diphenylurea; stroke treatment diphenylurea

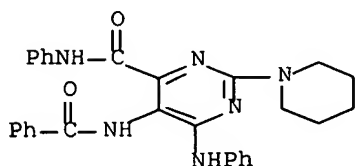
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 182700-31-8P

RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)  
 (preparation of N,N'-diphenylurea derivs. as interleukin-8 receptor  
 antagonists for disease treatment)

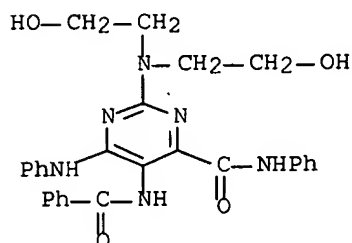
IT 182498-76-6P  
 RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)  
 (preparation of N,N'-diphenylurea derivs. as interleukin-8 receptor  
 antagonists for disease treatment)

RN 182498-76-6 HCAPLUS

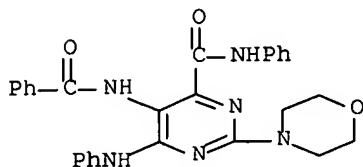
IT 59662-92-9 146073-99-6 146074-06-8  
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 (preparation and pharmacol. of aminopyrimidinecarboxylic acids)  
 IT 59662-97-4P 174805-11-9P 174805-12-0P  
 174805-13-1P 174805-14-2P 174805-15-3P  
 174805-16-4P 174805-17-5P 174805-18-6P  
 RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)  
 (preparation and pharmacol. of aminopyrimidinecarboxylic acids)  
 RN 59662-97-4 HCAPLUS  
 CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-N-phenyl-6-(phenylamino)-2-(1-  
 piperidinyl)- (CA INDEX NAME)



RN 174805-11-9 HCAPLUS  
 CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-2-[bis(2-hydroxyethyl)amino]-N-  
 phenyl-6-(phenylamino)- (CA INDEX NAME)



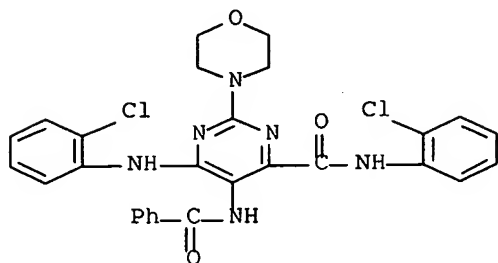
RN 174805-12-0 HCAPLUS  
 CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-2-(4-morpholinyl)-N-phenyl-6-  
 (phenylamino)- (CA INDEX NAME)



RN 174805-13-1 HCAPLUS  
 CN 4-Pyrimidinecarboxamide, 5-[(4-chlorobenzoyl)amino]-2-(4-morpholinyl)-N-  
 phenyl-6-(phenylamino)- (CA INDEX NAME)

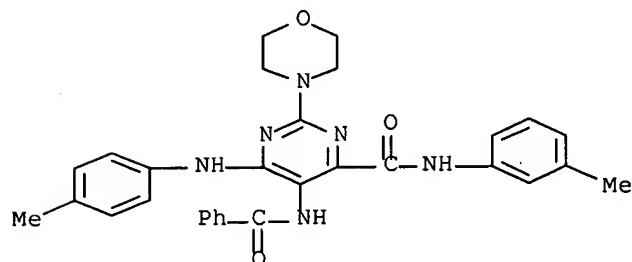
RN 174805-17-5 HCAPLUS

CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-N-(2-chlorophenyl)-6-[(2-chlorophenyl)amino]-2-(4-morpholinyl)- (CA INDEX NAME)



RN 174805-18-6 HCAPLUS

CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-N-(3-methylphenyl)-6-[(4-methylphenyl)amino]-2-(4-morpholinyl)- (CA INDEX NAME)



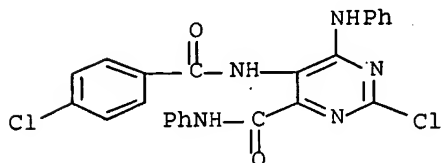
IT 146073-96-3

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation and pharmacol. of aminopyrimidinecarboxylic acids)

RN 146073-96-3 HCAPLUS

CN 4-Pyrimidinecarboxamide, 2-chloro-5-[(4-chlorobenzoyl)amino]-N-phenyl-6-(phenylamino)- (CA INDEX NAME)



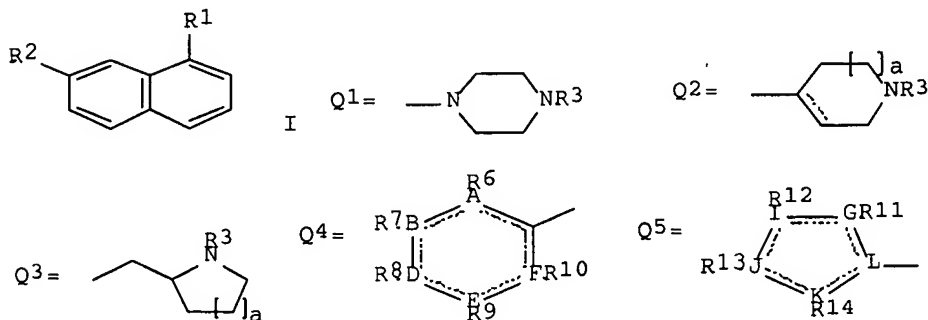
IT 59662-92-9 146073-99-6 146074-06-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and pharmacol. of aminopyrimidinecarboxylic acids)

PATENT ASSIGNEE(S): Barbara E.  
 SOURCE: Pfizer Inc., USA  
 PCT Int. Appl., 85 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9421619	A1	19940929	WO 1994-US1206	19940215 <--
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CA 2158457	C	20010417		
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GR 3036394	T3	20011130	GR 2001-401250	20010814 <--
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US 2005080090	A1	20050414	US 2003-645121	20030821 <--
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			WO 1994-US1206	W 19940215 <--
			US 1995-522349	B1 19950915 <--
			US 2001-758074	A1 20010110
			US 2001-4990	B1 20011203
OTHER SOURCE(S):				
MARPAT 122:314570				
GI				



AB Title compds. [I; R1 = Q1-Q3, etc.; R2 = R4, OR4, OS(O)2R4, NR4R5, R4(CH2)bNH(C:X)(CH2)c, R4(CH2)bo(C:O)NH(CH2)c(C:O)NH, R4(C:O)NH(C:O)NH, (CH2)bNH(C:X)(CH2)bo(C:O)(CH2)cR4, NH(C:X)NHR4, R4O(C:O)O, O(C:O)NHR4, R4O(C:O)NH, (CH2)b(C:O)(CH2)cR4, NHS(O)2R4, C(OH)R4R5, CH(OH)R4, (C:O)NR4R5, CN, NO2, substituted alkyl, (substituted) alkenyl, alkynyl; R3 = H, alkyl,

163498-50-8P 163498-82-6P 163498-83-7P 163498-84-8P 163498-85-9P  
 163498-86-0P 163498-87-1P 163498-88-2P 163498-89-3P 163498-90-6P  
 163498-91-7P 163531-32-6P

RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(preparation of heterocyclylnaphthalene derivs. as serotonin 5-HT1 agonists  
 and antagonists)

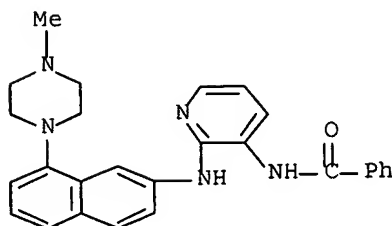
IT 163465-20-1P

RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(preparation of heterocyclylnaphthalene derivs. as serotonin 5-HT1 agonists  
 and antagonists)

RN 163465-20-1 HCAPLUS

CN Benzamide, N-[2-[[8-(4-methyl-1-piperazinyl)-2-naphthalenyl]amino]-3-  
 pyridinyl]- (CA INDEX NAME)



L163 ANSWER 38 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1993:116216 HCAPLUS Full-text

DOCUMENT NUMBER: 118:116216

TITLE: Synthesis and pharmacological properties of  
 2,4-disubstituted 5-amino-6-pyrimidinecarboxylic acid  
 derivatives. Part II

AUTHOR(S): Jasztold-Howorko, Ryszard; Machon, Zdzislaw;  
 Wilimowski, Marian; Wojewodzki, Wieslaw; Barczynska,  
 Jadwiga; Kedzierska, Lidia; Orzechowska-Juzwenko,  
 Krystyna; Dus, Ewa; Rutkowska, Maria; Szelag, Adam

CORPORATE SOURCE: Dep. Org. Chem., Med. Acad., Wroclaw, 50-137, Pol.

SOURCE: Polish Journal of Pharmacology and Pharmacy (

1992), 44(4), 393-406

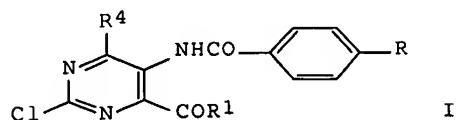
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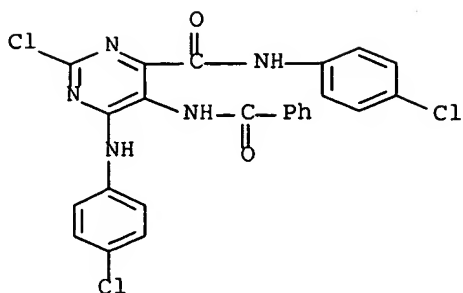
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 118:116216

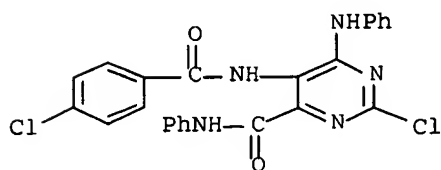
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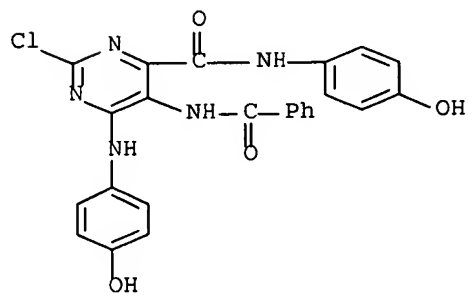
RN 146073-96-3 HCAPLUS

CN 4-Pyrimidinecarboxamide, 2-chloro-5-[(4-chlorobenzoyl)amino]-N-phenyl-6-(phenylamino)- (CA INDEX NAME)



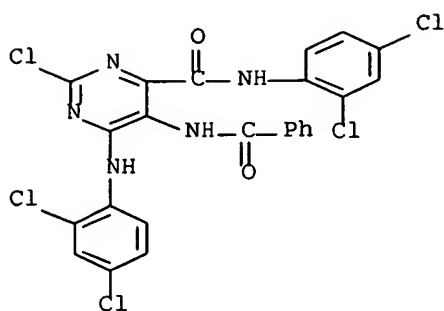
RN 146073-97-4 HCAPLUS

CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-2-chloro-N-(4-hydroxyphenyl)-6-[(4-hydroxyphenyl)amino]- (CA INDEX NAME)



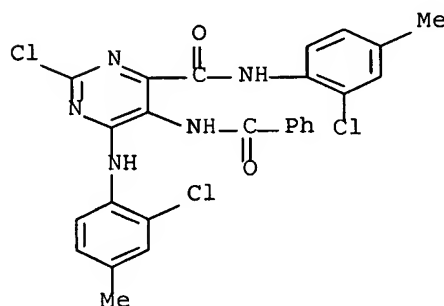
RN 146073-98-5 HCAPLUS

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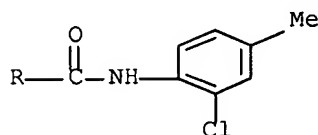
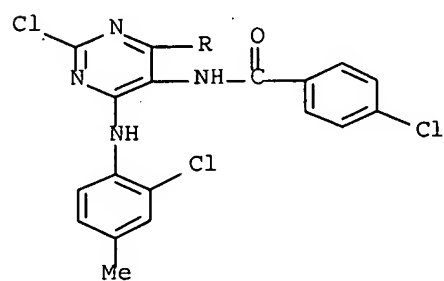
RN 146074-02-4 HCAPLUS

CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-2-chloro-N-(2-chloro-4-methylphenyl)-6-[(2-chloro-4-methylphenyl)amino]- (CA INDEX NAME)



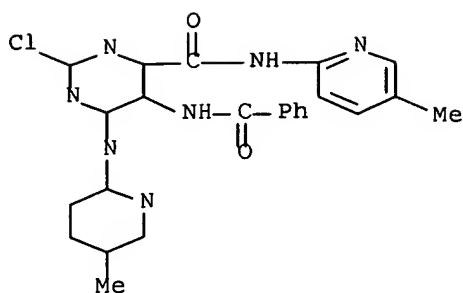
RN 146074-03-5 HCAPLUS

CN 4-Pyrimidinecarboxamide, 2-chloro-5-[(4-chlorobenzoyl)amino]-N-(2-chloro-4-methylphenyl)-6-[(2-chloro-4-methylphenyl)amino]- (CA INDEX NAME)



RN 146074-04-6 HCAPLUS

CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-2-chloro-N-(2-methylphenyl)-6-[(2-methylphenyl)amino]- (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L163 ANSWER 39 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:157882 HCAPLUS Full-text

DOCUMENT NUMBER: 112:157882

TITLE: N-Cycloalkylaminoethylbenzamide derivatives, their synthesis and pharmaceutical preparations

INVENTOR(S): Poli, Stefano; Coppi, Germano; Del Corona, Lucio

PATENT ASSIGNEE(S): Poli Industria Chimica S.p.A., Italy

SOURCE: Eur. Pat. Appl., 7 pp.

CODEN: EPXXDW

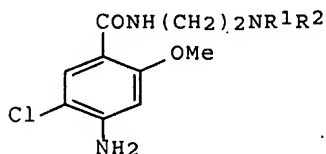
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 333073	A2	19890920	EP 1989-104315	19890310 <--
EP 333073	A3	19900912		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 5010108	A	19910423	US 1989-324596	19890315 <--
JP 02022257	A	19900125	JP 1989-64895	19890316 <--
PRIORITY APPLN. INFO.:			IT 1988-19814	A 19880317 <--
OTHER SOURCE(S):	MARPAT 112:157882			
GI				



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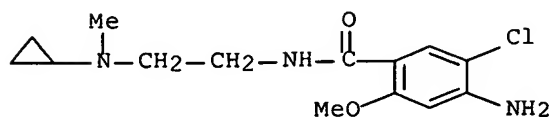
AB Title compds. I (R1 = H, alkyl, aralkyl; R2 = cycloalkyl) are prepared by acylation of R1R2N(CH2)NH2 with the corresponding benzoic acid (II). I are useful for treating gastritis, headaches, digestion troubles, psychosomatic disturbances in anxious subjects, nausea, and vomiting. II in THF was successively treated with carbonyldiimidazole and cyclopropylethylenediamine to give I (R1 = H; R2 = cyclopropyl), which at 0.27 mg/kg increased gastric transit rate by 50%.

IC ICM C07C103-82

ICS C07C102-04; A61K031-165



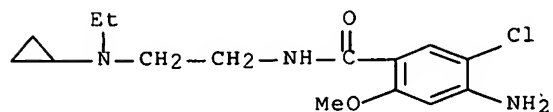
CN Benzamide, 4-amino-5-chloro-N-[2-(cyclopropylmethylamino)ethyl]-2-methoxy-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

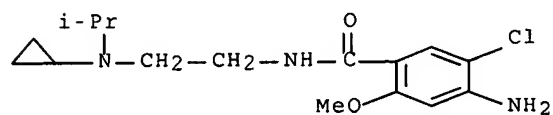
RN 126105-19-9 HCAPLUS

CN Benzamide, 4-amino-5-chloro-N-[2-(cyclopropylethylamino)ethyl]-2-methoxy-, (CA INDEX NAME)



RN 126105-20-2 HCAPLUS

CN Benzamide, 4-amino-5-chloro-N-[2-[cyclopropyl(1-methylethyl)amino]ethyl]-2-methoxy-, (CA INDEX NAME)



- AB Peptidomimetics of cyclic peptides, and compns. comprising such peptidomimetics are provided. The peptidomimetics have a three-dimensional structure that is substantially similar to a three-dimensional structure of a cyclic peptide that comprises a cadherin cell adhesion recognition sequence HAV. Methods for using such peptidomimetics for modulating cadherin-mediated cell adhesion in a variety of contexts are also provided.
- IC ICM A61K038-00
- INCL 514009000
- CC 1-3 (Pharmacology)  
Section cross-reference(s): 34, 63
- IT Angiogenesis inhibitors  
Antitumor agents  
Bladder, neoplasm  
Bond angle  
Cell migration  
Combinatorial library  
Conformation  
Drug delivery systems  
Drug screening  
Electrostatic charge  
Human  
Hydrophobicity  
Immunomodulators  
Melanoma  
Molecular modeling  
Multiple sclerosis  
Ovary, neoplasm  
Peptidomimetics  
Protein sequences  
QSAR (quantitative structure-activity relationship)  
Steric effects  
Transplant and Transplantation  
Wound healing  
Wound healing promoters  
(peptidomimetic modulators of cadherin-mediated cell adhesion for therapeutic use in relation to three-dimensional structure)
- IT 57-88-5D, Cholest-5-en-3-ol (3 $\beta$ )-, glycoside derivs. 135-16-0,  
L-Glutamic acid, N-[4-[(2-amino-1,4,5,6,7,8-hexahydro-4-oxo-6-pteridiny]methyl]amino]benzoyl]- 487-49-0, Ethanone, 1-(2,4-dihydroxyphenyl)-2-(4-methoxyphenyl)- 548-73-2, 2H-Benzimidazol-2-one, 1-[1-[4-(4-fluorophenyl)-4-oxobutyl]-1,2,3,6-tetrahydro-4-pyridinyl]-1,3-dihydro- 570-88-7, Cholest-4-ene-3,6-diol, (3 $\beta$ ,6 $\beta$ )- 1210-66-8, 1H-Purin-6-amine, N-phenyl- 1482-74-2, 2-Propen-1-one, 3-phenyl-1-(2,3,4-trihydroxyphenyl)- 1699-40-7, Benzeneacetamide, 4-methoxy-N-[2-[3-methoxy-4-(phenylmethoxy)phenyl]ethyl]-3-(phenylmethoxy)- 1776-30-3, 2-Propen-1-one, 1-(2,4-dihydroxyphenyl)-3-phenyl- 2486-02-4, Benzoic acid, 3,4,5-trihydroxy-, 3-methylbutyl ester 2810-37-9, 1H-Isoindole-1,3(2H)-dione, 2-[5-(1H-benzotriazol-1-yl)propyl]- 2979-51-3, 1H-Imidazole, 1-(1-oxo-3-phenyl-2-propenyl)- 3242-68-0, L-Glutamic acid, N-[4-[[2-[(2-amino-1,4-dihydro-4-oxo-5-pyrimidinyl)amino]ethyl]amino]benzoyl]- 3257-73-6, 9H-Purin-6-amine, 9-[2,3,5-tris-O-(phenylmethyl)- $\beta$ -D-arabinofuranosyl]- 3561-56-6, L-Asparagine, N2-[(phenylmethoxy)carbonyl]-, (4-nitrophenyl)methyl ester 3566-25-4, L-Glutamic acid, N-[4-[[2-(2-amino-1,4-dihydro-4-oxo-6-pteridiny]ethyl]amino]benzoyl]- 3575-07-3, 1H-Benzimidazole, 2,2'-(1,2-ethanediyl)bis- 3922-47-2, 1H-1,2,4-Triazol-3-amine, 5-[(phenylmethyl)thio]- 4672-96-2, Benzeneacetamide, 3-methoxy-N-[2-[4-methoxy-3-(phenylmethoxy)phenyl]ethyl]-4-(phenylmethoxy)- 5226-71-1, Benzene, 1,1'-[1,10-decanediylbis(oxy)]bis[3-nitro-

1]-, diethyl ester 27430-15-5, 4,6(1H,5H)-Pyrimidinedione, 5-[[4-(dimethylamino)phenyl]methylene]dihydro-2-thioxo- 27430-17-7, 4,6(1H,5H)-Pyrimidinedione, dihydro-5-(3-phenyl-2-propenylidene)-2-thioxo- 28005-33-6, Benzene, 1,1'-methylenebis[4-[(4-nitrophenyl)thio]- 28246-23-3, Ethanone, 2-(1H-imidazol-2-ylthio)-1-phenyl- 28772-56-7, 2H-1-Benzopyran-2-one, 3-[3-(4'-bromo[1,1'-biphenyl]-4-yl)-3-hydroxy-1-phenylpropyl]-4-hydroxy- 29654-52-2, Benzene, 1,1'-methylenebis[4-[(4-nitrophenyl)sulfonyl]- 30148-18-6, Methanone, (4-chlorophenyl)(1-methyl-1H-imidazol-2-yl)- 30216-31-0D, Benzoxazole, 2-[2-(2-chlorophenyl)ethenyl]-, derivs. 30355-60-3, 1,3,5-Triazine-2,4-diamine, 6-(chloromethyl)-N-phenyl- 30826-46-1, L-Glutamic acid, N-[4-[[[5,7-bis(acetylamino)pyrido[3,4-b]pyrazin-3-yl)methyl]methylamino]benzoyl]-, diethyl ester 30826-47-2, L-Glutamic acid, N-[4-[[[6,8-bis(acetylamino)pyrido[2,3-b]pyrazin-2-yl)methyl]methylamino]benzoyl]-, diethyl ester 33254-46-5, 6H-Purine-6-thione, 1,9-dihydro-9-(3-phenylpropyl)- 34396-76-4, 6H-Purin-6-one, 1,9-dihydro-9-(3-phenylpropyl)- 37664-31-6, Ethanone, 1-(4-chlorophenyl)-2-(1H-1,2,4-triazol-3-ylthio)- 40538-65-6, 5(4H)-Isoxazolone, 3-methyl-4-[(phenylamino)methylene]- 40816-36-2, 4,6-Pyrimidinediamine, 5-nitro-N-phenyl- 41266-78-8, 1H-1,2,4-Triazol-3-amine, 5-[[4-(chlorophenyl)methyl]thio]- 41600-13-9, L-Glutamic acid, N-[4-[[[2,4-diamino-6-pteridiny]methyl]methylamino]benzoyl]-L-γ-glutamyl- 42220-83-7, 2-Propen-1-one, 1-(2,4-dihydroxyphenyl)-3-(3-hydroxyphenyl)- 46825-86-9, Pyrimidinetetramine, N4-(4-bromophenyl)- 50602-77-2, L-Glutamic acid, N-[4-[[[2,4-diamino-6-pteridiny]methyl]methylamino]benzoyl]-, dibutyl ester 51646-15-2, [1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[(phenylmethyl)thio]- 51893-98-2, Benzoic acid, 2-hydroxy-, [2-[(5-ethyl-1,4-dihydro-6-methyl-4-oxo-2-pyrimidinyl)thio]-1-phenylethylidene]hydrazide 51934-26-0, L-Glutamic acid, N-[4-[[[7-amino-1,5-dihydro-5-thioxopyrimido[5,4-e]-1,2,4-triazin-3-yl)methyl]amino]benzoyl]-, diethyl ester, monohydrochloride 51934-28-2, L-Glutamic acid, N-[4-[[[5,7-diaminopyrimido[5,4-e]-1,2,4-triazin-3-yl)methyl]amino]benzoyl]-, diethyl ester 54299-50-2, 2-Propen-1-one, 1-(2,4-dihydroxy-3,6-dimethoxyphenyl)-3-phenyl- 54395-52-7, 1H-Isoindole-1,3(2H)-dione, 5,5'-[(1-methylethylidene)bis(4,1-phenyleneoxy)]bis[2-methyl- 56025-86-6, 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-(phenylmethyl)- 56307-99-4, Ethanone, 1-(2,4-dihydroxyphenyl)-2-(phenylthio)- 57710-80-2, 1H-Benzotriazole-1-carboxylic acid, phenylmethyl ester 57808-66-9, 2H-Benzimidazol-2-one, 5-chloro-1-[1-[3-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)propyl]-4-piperidinyl]-1,3-dihydro- 57966-42-4, L-Threonine, L-arginyl-L-tyrosyl-L-leucyl-L-prolyl- 58677-09-1, L-Glutamic acid, N-[4-[[[2-amino-1,4-dihydro-4-oxo-6-quinazolinyl)methyl]methylamino]benzoyl]-, diethyl ester 60045-61-6, 4,6(1H,5H)-Pyrimidinedione, dihydro-5-[(4-methoxyphenyl)methylene]-2-thioxo- 60407-48-9, L-Isoleucine, L-arginylglycyl-L-prolyl-L-phenylalanyl-L-prolyl- 60482-96-4, L-Leucine, L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- 61043-53-6, L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-alanyl-N-(4-nitrophenyl)- 64792-21-8, 2-Propenal, 3-phenyl-, (1,4-dihydro-6-methyl-4-oxo-2-pyrimidinyl)hydrazone 64801-58-7, L-Aspartic acid, N-[4-[[[2,4-diamino-6-pteridiny]methyl]methylamino]benzoyl]-L-γ-glutamyl- 65147-09-3, L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L-leucylglycyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)- 65757-04-2, L-Glutamic acid, N-[4-[[[1,2,3,4-tetrahydro-2-imino-1,3-dimethyl-4-oxo-6-pteridiny]methyl]amino]benzoyl]-, dimethyl ester 65757-05-3, L-Glutamic acid, N-[4-[[[2-amino-3,4-dihydro-3-methyl-4-oxo-6-pteridiny]methyl]amino]benzoyl]-, dimethyl ester 65877-43-2D, 1,3-Benzenediol, 5-[2-(3-hydroxy-4-methoxyphenyl)ethenyl]-, glycoside derivative 66048-53-1, Guanosine, 2',3',5'-tribenzoate 66147-31-7, L-Glutamic acid, N-[4-[[[2,4-diamino-6-pteridiny]methyl]methylamino]benzo

1-acetyl-L-prolyl-L-leucylglycyl-L-leucyl-L-leucyl-, ethyl ester  
 93515-01-6, L-Threonine, L-tyrosyl-L-prolyl-L-prolyl-L- $\alpha$ -glutamyl-L-prolyl-L- $\alpha$ -glutamyl- 93524-30-2,  $\beta$ -D-Glucopyranosiduronic acid, (3 $\alpha$ ,5 $\beta$ )-21-(acetyloxy)-20-[(aminocarbonyl)hydrazono]pregnan-3-yl, methyl ester, 2,3,4-triacetate 93674-97-6, L-Serine, L-arginylglycyl-L- $\alpha$ -glutamyl- 95192-21-5, L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-phenylalanyl-L-alanyl-N-(4-nitrophenyl)- 95192-38-4, L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-valyl-L-prolyl-N-(4-nitrophenyl)- 95210-75-6, L-Proline, L-tyrosyl-L-prolyl-L-phenylalanyl-L-valyl-L- $\alpha$ -glutamyl-L-prolyl-L-isoleucyl- 98018-39-4, Ethanone, 2-[(2-amino-1H-purin-6-yl)thio]-1-phenyl- 98151-93-0, L-Proline, L-tyrosyl-L-prolyl-L-phenylalanyl-L-prolylglycyl-L-prolyl-L-isoleucyl- 100975-56-2, Benzaldehyde, 4-hydroxy-, (2,3,6,7-tetrahydro-1,3,7-trimethyl-2,6-dioxo-1H-purin-8-yl)hydrazone 102212-40-8, 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-[(2-phenylethyl)amino]- 103030-49-5, 2,4-Pyrimidinediamine, N4-(4-chlorophenyl)-5-nitro- 103398-43-2, Benzenemethanol, 2-[bis[2-[(4-nitrobenzoyl)oxy]ethyl]amino]-, 4-nitrobenzoate (ester) 105037-36-3, Benzenesulfonic acid, 4-[(7-chloro-4-quinazolinyl)amino]- 108608-63-5, Glycine, L-seryl-L- $\alpha$ -aspartylglycyl-L-arginyl- 110906-89-3, L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-phenylalanyl-L-alanyl-L-alanyl-N-(4-nitrophenyl)- 111172-14-6, 1,3-Benzodioxole-5-carboxaldehyde, O-(2-thienylcarbonyl)oxime 112233-74-6, Carbamic acid, diphenyl-, 2-(acetyl-amino)-1H-purin-6-yl ester 113866-00-5, L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L- $\alpha$ -aspartyl-L-prolyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)-, phenylmethyl ester 113866-16-3, L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L- $\alpha$ -glutamyl-L-alanyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)-, phenylmethyl ester 117889-48-2, 1H-Tetrazole, 5-[(2,4-dichlorophenoxy)methyl]- 118034-92-7, L-Threonine, L-histidyl-L-phenylalanyl-L-methionyl-L-prolyl- 120225-54-9, Benzenepropanoic acid, 4-[2-[[6-amino-9-(N-ethyl- $\beta$ -D-ribofuranuronamidoyl)-9H-purin-2-yl]amino]ethyl]- 121036-80-4, 1,2,4-Triazin-5(2H)-one, 6-[2-(4-methylphenyl)ethenyl]-3-phenyl- 121036-81-5, 1,2,4-Triazin-5(2H)-one, 6-[2-(4-methoxyphenyl)ethenyl]-3-phenyl- 124485-41-2, L-Argininamide, N-[(phenylmethoxy)carbonyl]-L-valyl-L-valyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)- 126235-09-4, 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(2-phenylethyl)- 128802-79-9, L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-isoleucyl-L-prolyl-N-(4-nitrophenyl)- 131061-65-9, 7H-Purine-7-butanoic acid, 1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-8-[(phenylmethyl)amino]-, ethyl ester 132467-01-7, 2(1H)-Quinoxalinone, 3-[2-(2-chlorophenyl)ethenyl]- 133061-57-1, 2,4-Pyrimidinediamine, N4-(3,5-dichlorophenyl)-6-methyl- 134759-22-1, 1H-Thieno[3,4-d]imidazole-4-pentanamide, N-[6-[[5-[[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9']-[9H]xanthen]-5-yl)amino]thioxomethyl]amino]pentyl]amino]-6-oxohexyl]hexahydro-2-oxo-, (3aS,4S,6aR)- 134796-34-2, 1H-1,2,4-Triazole, 3-[[[(4-chlorophenyl)methyl]thio]- 137484-84-5, 1,3,5-Triazin-2-amine, 4-chloro-6-[3-(2-furanyl)propoxy]-N,N-dimethyl- 137833-31-9, Myelopeptide 2 138194-56-6, 1H-Pyrrole-2,5-dione, 1-[3-[[[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)oxy]carbonyl]phenyl]- 138915-75-0, L-Leucine, N-acetyl-L-histidyl-L-tryptophyl-L-alanyl-L-valylglycyl-L-histidyl- 142206-40-4, 1H-Benzimidazole, 2,2'-(1,3-propanediyl)bis[1-methyl- 143113-41-1, L-Valine, L-Histidyl-L-Alanyl 146871-70-7, 4-Quinazolinamine, N-(3-chlorophenyl)-, monohydrochloride 148337-06-8, Glycine, L-prolylglycyl-L-alanyl-L-isoleucyl-L-prolyl- 151358-70-2, 2-Propen-1-one, 1,1'-(2,6-pyridinediyl)bis[3-(4-hydroxyphenyl)- 152028-96-1, 1H-Imidazole, 4-[3-[(4-iodophenyl)methoxy]propyl]- 154719-25-2, L-Lysinamide, N-acetyl-L-tyrosyl-L-valyl-N-[(1S)-1-(carboxymethyl)-3-[(2,6-dimethylbenzoyl)oxy]-2-oxopropyl]-N6-[5-

L164 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2002:869496 HCAPLUS Full-text  
 DOCUMENT NUMBER: 137:363033  
 TITLE: Peptidomimetic modulators of cell adhesion  
 INVENTOR(S): Gour, Barbara J.; Blaschuk, Orest W.; Ali, Anmar; Ni, Feng; Chen, Zhigang; Michaud, Stephanie D.; Wang, Shoameng; Hu, Zenjian  
 PATENT ASSIGNEE(S): Can.  
 SOURCE: U.S. Pat. Appl. Publ., 309 pp., Cont.-in-part of U.S. Ser. No. 491,078.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 15  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002168761	A1	20021114	US 2001-769145	20010124 <--
US 2004058864	A1	20040325	US 2003-412701	20030410 <--
US 7268115	B2	20070911		
US 2004006011	A1	20040108	US 2003-425557	20030428 <--
PRIORITY APPLN. INFO.:			US 2000-491078	A2 20000124 <--
			US 1996-21612P	P 19960712 <--
			US 1997-893534	A1 19970711 <--
			US 2000-507102	A1 20000217 <--
			US 2001-769145	B1 20010124
			US 2001-6982	A2 20011204

OTHER SOURCE(S): MARPAT 137:363033

AB Peptidomimetics of cyclic peptides, and compns. comprising such peptidomimetics are provided. The peptidomimetics have a three-dimensional structure that is substantially similar to a three-dimensional structure of a cyclic peptide that comprises a cadherin cell adhesion recognition sequence HAV. Methods for using such peptidomimetics for modulating cadherin-mediated cell adhesion in a variety of contexts are also provided.

IC ICM A61K038-17  
 ICS C07K014-435; C12N005-02

INCL 435325000

CC 1-3 (Pharmacology)  
 Section cross-reference(s): 34, 63

IT Angiogenesis inhibitors  
 Antitumor agents  
 Bladder, neoplasm  
 Bond angle  
 Cell migration  
 Combinatorial library  
 Conformation  
 Drug delivery systems  
 Drug delivery systems  
 Drug screening  
 Electrostatic charge  
 Human  
 Hydrophobicity  
 Immunomodulators  
 Melanoma  
 Molecular modeling  
 Multiple sclerosis

acid, N-[4-[[[(2-amino-1,4-dihydro-4-oxo-6-pteridiny]methyl]amino]benzoyl]-  
L- $\alpha$ -glutamyl- 6962-62-5, 2-Propen-1-one, 3-(1,3-benzodioxol-5-yl)-  
1-(2,4-dihydroxyphenyl)- 6975-34-4, 1H-Purine, 6-[(3-phenyl-2-  
propenyl)thio]- 7781-29-5, 2,4-Pyrimidinediamine, 6-methyl-N4-phenyl-  
10320-97-5, 1,2,3,4-Thiatriazol-5-amine, N-1-naphthalenyl- 13184-14-0,  
L-Lysine, L-lysyl-L-lysyl- 13351-10-5, 2-Propen-1-one,  
1-(2,4-dihydroxyphenyl)-3-(4-methoxyphenyl)- 13745-20-5, 2-Propen-1-one,  
1-(2,4-dihydroxyphenyl)-3-(4-hydroxyphenyl)- 15013-60-2,  
Cholest-4-ene-3,6-diol, (3 $\beta$ ,6 $\alpha$ )- 15970-42-0,  
1H-Imidazole-1,2-diamine, 4-(4-chlorophenyl)- 16856-21-6, L-Tryptophan,  
N-[N-[(phenylmethoxy)carbonyl]-L-phenylalanyl]-, methyl ester  
16879-84-8, L-Threonine, N-[(phenylmethoxy)carbonyl]-,  
(4-nitrophenyl)methyl ester 17357-75-4, 1H-1,2,4-Triazole,  
3-[[[(4-methoxyphenyl)methyl]thio]- 17430-65-8, L-Tryptophan,  
N-[(phenylmethoxy)carbonyl]-L-valyl-, methyl ester 17496-31-0,  
1H-Imidazole, 4-[[[(phenylmethyl)thio]methyl]- 18100-11-3,  
1,4-Naphthalenedione, 2-(3-cyclohexylbutyl)-3-hydroxy- 18100-12-4,  
1,4-Naphthalenedione, 2-[3-(4-chlorophenyl)propyl]-3-hydroxy-  
18211-37-5, 1,4-Naphthalenedione, 2-hydroxy-3-[3-(4-methylphenyl)propyl]-  
19312-13-1, 2-Propen-1-one, 1-(2,5-dihydroxyphenyl)-3-phenyl-  
19484-75-4D, 2H-1-Benzopyran-2-one, 3,4-dihydro-7-hydroxy-4-methyl-,  
furanoside derivative 19889-31-7, 1H-Imidazole-4-propanamide,  
 $\alpha$ -amino-N-2-naphthalenyl- 20621-49-2, 2-Propen-1-one,  
1-(2,6-dihydroxy-4-methoxyphenyl)-3-(4-methoxyphenyl)- 21108-76-9,  
Imidazo[2,1-b]thiazol-3(2H)-one, 5,6-dihydro-2-(3-phenyl-2-propenylidene)-  
21658-45-7, Glycine, L-arginyl-L-prolyl-L-prolyl- 23567-67-1, Phenol,  
4-(1,2,3,4-thiatriazol-5-ylamino)- 23815-88-5, 1-6-Bradykinin  
24205-32-1, L-Glutamic acid, N-[4-[[[(2,4-diamino-5-methyl-6-  
quinazolinyl)methyl]amino]benzoyl]-, diethylester 24386-39-8, Urea,  
N-1-naphthalenyl-N'-2-pyrimidinyl- 24829-12-7, Phenol,  
2-[(1H-1,2,4-triazol-3-ylimino)methyl]- 26962-50-5, 2-Propen-1-one,  
1-(2,4-dihydroxyphenyl)-3-(2-hydroxyphenyl)- 27069-81-4, L-Glutamic  
acid, N-[4-[[[(2-amino-1,4-dihydro-4-oxo-6-quinazolinyl)methyl]amino]benzoyl]-,  
diethyl ester 27430-15-5, 4,6(1H,5H)-Pyrimidinedione,  
5-[[4-(dimethylamino)phenyl]methylene]dihydro-2-thioxo- 27430-17-7,  
4,6(1H,5H)-Pyrimidinedione, dihydro-5-(3-phenyl-2-propenylidene)-2-thioxo-  
28005-33-6, Benzene, 1,1'-methylenebis[4-[(4-nitrophenyl)thio]-  
28246-23-3, Ethanone, 2-(1H-imidazol-2-ylthio)-1-phenyl- 28772-56-7,  
2H-1-Benzopyran-2-one, 3-[3-(4'-bromo[1,1'-biphenyl]-4-yl)-3-hydroxy-1-  
phenylpropyl]-4-hydroxy- 29654-52-2, Benzene, 1,1'-methylenebis[4-[(4-  
nitrophenyl)sulfonyl]- 30148-18-6, Methanone, (4-chlorophenyl)(1-methyl-  
1H-imidazol-2-yl)- 30216-31-0D, Benzoxazole, 2-[2-(2-  
chlorophenyl)ethenyl]-, derivs. 30355-60-3, 1,3,5-Triazine-2,4-diamine,  
6-(chloromethyl)-N-phenyl- 30826-46-1, L-Glutamic acid,  
N-[4-[[[5,7-bis(acetylamino)pyrido[3,4-b]pyrazin-3-  
yl]methyl]methylamino]benzoyl]-, diethyl ester 30826-47-2, L-Glutamic  
acid, N-[4-[[[6,8-bis(acetylamino)pyrido[2,3-b]pyrazin-2-  
yl]methyl]methylamino]benzoyl]-, diethyl ester 33254-46-5,  
6H-Purine-6-thione, 1,9-dihydro-9-(3-phenylpropyl)- 34396-76-4,  
6H-Purin-6-one, 1,9-dihydro-9-(3-phenylpropyl)- 37664-31-6, Ethanone,  
1-(4-chlorophenyl)-2-(1H-1,2,4-triazol-3-ylthio)- 40538-65-6,  
5(4H)-Isoxazolone, 3-methyl-4-[(phenylamino)methylene]- 40816-36-2,  
4,6-Pyrimidinediamine, 5-nitro-N-phenyl- 41266-78-8,  
1H-1,2,4-Triazol-3-amine, 5-[[[(4-chlorophenyl)methyl]thio]- 41600-13-9,  
L-Glutamic acid, N-[4-[[[(2,4-diamino-6-pteridiny]methyl]methylamino]benzo  
yl]-L- $\gamma$ -glutamyl- 42220-83-7, 2-Propen-1-one, 1-(2,4-  
dihydroxyphenyl)-3-(3-hydroxyphenyl)- 46825-86-9, Pyrimidinetetramine,  
N4-(4-bromophenyl)- 50602-77-2, L-Glutamic acid, N-[4-[[[(2,4-diamino-6-  
pteridiny]methyl]methylamino]benzoyl]-, dibutyl ester 51646-15-2,

pteridiny]methyl]amino]benzoyl]-L- $\gamma$ -glutamyl]- 72630-15-0,  
 Glutamic acid, N-[4-[[2-(2-amino-1,4,5,6,7,8-hexahydro-5-methyl-4-oxo-6-  
 pteridiny]ethyl]amino]benzoyl]- 72682-77-0, L-Isoleucinamide,  
 N-(3-carboxy-1-oxopropyl)-L-alanyl-L-alanyl-L-prolyl-N-(4-nitrophenyl)-  
 72704-76-8, 2-Propen-1-one, 3-(3,4-dihydroxyphenyl)-1-phenyl-  
 73554-90-2, L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L-  
 phenylalanyl-L-seryl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)-  
 73572-58-4, L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-L-  
 phenylalanyl-L-leucyl-L-phenylalanyl-L-leucyl- 74039-67-1,  
 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(3-phenyl-2-propenyl)-  
 74405-42-8, Adenosine, N-benzoyl-5'-O-[bis(4-methoxyphenyl)phenylmethyl]-  
 2'-deoxy-, 3'-(hydrogen butanedioate) 74405-44-0, Cytidine,  
 N-benzoyl-5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-, 3'-(hydrogen  
 butanedioate) 74853-69-3, L-Leucine, N2-acetyl-L-arginyl-L-arginyl-L-  
 prolyl-L-tyrosyl-L-isoleucyl- 75651-68-2, L-Phenylalaninamide,  
 N-(3-carboxy-1-oxopropyl)-L-phenylalanyl-L-prolyl-N-(4-nitrophenyl)-  
 75960-43-9, 1H-Imidazole-4-hexanoic acid, 5-(chloromethyl)-2,3-dihydro-  
 $\epsilon$ ,2-dioxo-, ethyl ester 76172-68-4, i-Propanone,  
 3-(4-methoxyphenyl)-1-(2,4,6-trihydroxyphenyl)- 80032-99-1,  
 1H-1,2,4-Triazole, 3,3'-[1,4-butanediylbis(thio)]bis- 80360-08-3,  
 L-Glutamic acid, N-[4-[[[(2,4-diaminopyrido[2,3-d]pyrimidin-6-  
 yl)methyl]amino]benzoyl]-, diethyl ester 81066-61-7, 2-Pyridinamine,  
 3-[[4-(1,1-dimethylethyl)phenyl]methoxy]- 81587-37-3, 3-Pyridinethiol,  
 2-[(2,6-diamino-4-pyrimidinyl)amino]-6-methyl- 82628-82-8, 1-Propanone,  
 3-(4-nitrophenyl)-1-(2,4,6-trihydroxyphenyl)- 82855-85-4, L-Glutamic  
 acid, N-[4-[[[(2-amino-1,4,5,6,7,8-hexahydro-4-oxopyrido[3,2-d]pyrimidin-6-  
 yl)methyl]amino]benzoyl]-, diethyl ester 85122-85-6,  
 1H-Isoindole-1,3(2H)-dione, 2,2'-[1,3-propanediylbis(4,1-  
 piperidinediylmethylene)]bis- 86669-33-2, L-Glutamic acid,  
 N-[4-[[[(2,4-diamino-6-pteridiny]methyl)methylamino]benzoyl]-,  
 bis(1,1-dimethylethyl) ester 90259-60-2, Benzamide, 2-amino-N-[3-(1H-  
 imidazol-1-yl)propyl]- 90259-61-3, Benzamide, 2-[[4-(  
 chlorophenyl)sulfonyl]amino]-N-[3-(1H-imidazol-1-yl)propyl]- 92899-39-3,  
 Glycine, L-valylglycyl-L-valyl-L-alanyl-L-prolyl- 92954-99-9, Glycine,  
 1-acetyl-L-prolyl-L-leucylglycyl-L-leucyl-L-leucyl-, ethyl ester  
 93515-01-6, L-Threonine, L-tyrosyl-L-prolyl-L-prolyl-L- $\alpha$ -glutamyl-L-  
 prolyl-L- $\alpha$ -glutamyl- 93524-30-2,  $\beta$ -D-Glucopyranosiduronic  
 acid, (3 $\alpha$ ,5 $\beta$ )-21-(acetyloxy)-20-[(aminocarbonyl)hydrazono]pregn  
 an-3-yl, methyl ester, 2,3,4-triacetate 93674-97-6, L-Serine,  
 L-arginylglycyl-L- $\alpha$ -glutamyl- 95192-21-5, L-Phenylalaninamide,  
 N-(3-carboxy-1-oxopropyl)-L-phenylalanyl-L-alanyl-N-(4-nitrophenyl)-  
 95192-38-4, L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-  
 valyl-L-prolyl-N-(4-nitrophenyl)- 95210-75-6, L-Proline,  
 L-tyrosyl-L-prolyl-L-phenylalanyl-L-valyl-L- $\alpha$ -glutamyl-L-prolyl-L-  
 isoleucyl- 98018-39-4, Ethanone, 2-[(2-amino-1H-purin-6-yl)thio]-1-  
 phenyl- 98151-93-0, L-Proline, L-tyrosyl-L-prolyl-L-phenylalanyl-L-  
 prolylglycyl-L-prolyl-L-isoleucyl- 100975-56-2, Benzaldehyde,  
 4-hydroxy-, (2,3,6,7-tetrahydro-1,3,7-trimethyl-2,6-dioxo-1H-purin-8-  
 yl)hydrazone 102212-40-8, 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-  
 8-[(2-phenylethyl)amino]- 103030-49-5, 2,4-Pyrimidinediamine,  
 N4-(4-chlorophenyl)-5-nitro- 103398-43-2, Benzenemethanol,  
 2-[bis[2-[(4-nitrobenzoyl)oxy]ethyl]amino]-, 4-nitrobenzoate (ester)  
 105037-36-3, Benzenesulfonic acid, 4-[(7-chloro-4-quinazolinyl)amino]-  
 108608-63-5, Glycine, L-seryl-L- $\alpha$ -aspartylglycyl-L-arginyl-  
 110906-89-3, L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-phenylalanyl-  
 L-alanyl-L-alanyl-N-(4-nitrophenyl)- 111172-14-6, 1,3-Benzodioxole-5-  
 carboxaldehyde, O-(2-thienylcarbonyl)oxime 112233-74-6, Carbamic acid,  
 diphenyl-, 2-(acetyl-amino)-1H-purin-6-yl ester 113866-00-5,  
 L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L- $\alpha$ -aspartyl-L-

nitrophenyl)ethyl]imino]methyl]- 202118-27-2, 1H-1,2,4-Triazol-3-amine,  
 N-[(2-iodophenyl)methylene]- 202118-28-3, 1H-1,2,4-Triazol-3-amine,  
 N-[(2-chlorophenyl)methylene]- 202332-09-0, 1,4-Benzenediol,  
 2-(6-methylheptyl)- 202528-15-2, Cyclo(L-alanyl-L-histidyl-L-alanyl-L-  
 valyl-L- $\alpha$ -aspartyl-L-isoleucyl) 206360-24-9, 4H-1-Benzopyran-4-  
 one, 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-3-(3-methyl-2-butenyl)-  
 210709-22-1, L-Alanine, N2-benzoyl-L-arginyl-L-phenylalanyl-  
 215434-58-5, 1-Piperazinecarbothioamide, N-3-pyridinyl-4-[4-  
 (trifluoromethyl)-2-pyrimidinyl]- 215655-36-0, Benzoic acid,  
 2-[[[2-[[4-(trifluoromethyl)-2-pyrimidinyl]amino]ethyl]amino]carbonyl]-  
 215657-86-6, 2-Pyrrolidinone, 1-[2-hydroxy-3-[4-[4-(trifluoromethyl)-2-  
 pyrimidinyl]-1-piperazinyl]propyl]-

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);  
 PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES  
 (Uses)

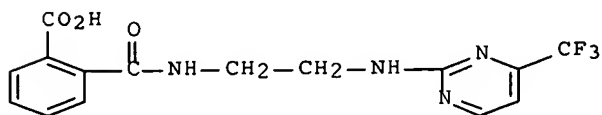
(peptidomimetic modulators of cadherin-mediated cell adhesion for  
 therapeutic use in relation to three-dimensional structure)

IT 215655-36-0, Benzoic acid, 2-[[[2-[[4-(trifluoromethyl)-2-  
 pyrimidinyl]amino]ethyl]amino]carbonyl]-  
 RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);  
 PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES  
 (Uses)

(peptidomimetic modulators of cadherin-mediated cell adhesion for  
 therapeutic use in relation to three-dimensional structure)

RN 215655-36-0 HCAPLUS

CN Benzoic acid, 2-[[[2-[[4-(trifluoromethyl)-2-pyrimidinyl]amino]ethyl]amino  
 ]carbonyl]- (CA INDEX NAME)



L164 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:545724 HCAPLUS Full-text

DOCUMENT NUMBER: 135:147398

TITLE: Peptidomimetic modulators of cell adhesion

INVENTOR(S): Gour, Barbara J.; Blaschuk, Orest W.; Ali, Anmar; Ni,  
 Feng; Chen, Zhigang; Michaud, Stephanie Denise; Wang,  
 Shoameng; Hu, Zengjian

PATENT ASSIGNEE(S): Adherex Technologies, Inc., Can.

SOURCE: PCT Int. Appl., 416 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 15

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001053331	A2	20010726	WO 2001-US2508	20010124 <--
WO 2001053331	A3	20020711		
WO 2001053331	A9	20021031		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,  
 CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,



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 138194-56-6 138915-75-0 142206-40-4 146871-70-7 148337-06-8  
 151358-70-2 152028-96-1 154719-25-2 155373-59-4 155373-72-1  
 160347-57-9D, derivs. 185503-97-3 188966-22-5D, derivs. 191411-47-9  
 194424-08-3 195140-70-6 196600-87-0 197456-56-7 198488-04-9  
 198632-08-5 199929-21-0 200058-34-0 200061-22-9 200431-98-7  
 200505-51-7 200706-30-5 200706-45-2 201997-13-9 202118-27-2  
 202118-28-3 202332-09-0 202528-15-2 206360-24-9 210709-22-1  
 215434-58-5 215655-36-0

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)

(peptidomimetic modulators of cell adhesion)

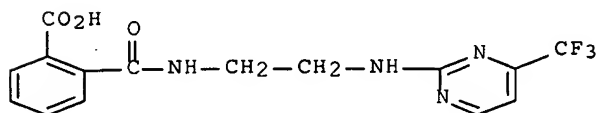
IT 215655-36-0

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)

(peptidomimetic modulators of cell adhesion)

RN 215655-36-0 HCAPLUS

CN Benzoic acid, 2-[[[2-[[4-(trifluoromethyl)-2-pyrimidinyl]amino]ethyl]amino]carbonyl]- (CA INDEX NAME)



L130 912 SEA FILE=HCAPLUS ABB=ON L94 AND (PY<2001 OR AY<2001 OR  
 PRY<2001)  
 L147 3612 SEA FILE=HCAPLUS ABB=ON (PAIN(3A)RECEPTOR#)/BI  
 L148 1 SEA FILE=HCAPLUS ABB=ON L147 AND L130

=> s l141,l146,l148 not l163,l96,l164

L165 9 (L141 OR L146 OR L148) NOT (L163 OR L96 OR L164)

=> d ibib abs hitind hitstr l165 1-9

L165 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:739839 HCAPLUS Full-text

DOCUMENT NUMBER: 141:256974

TITLE: Amplified luminescent homogeneous immunoassay

INVENTOR(S): Ullman, Edwin F.; Singh, Rajendra; De Keczer, Steve;  
 Davalian, Dariush

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 71 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 2004175696	A1	20040909	US 2000-732047	20001207 <--
PRIORITY APPLN. INFO.:			US 2000-732047	20001207 <--
OTHER SOURCE(S):	MARPAT	141:256974		

AB Methods are disclosed for determining minute quantities of an analyte in a medium suspected of containing the analyte. One method comprises treating a medium suspected of containing an analyte under conditions such that the analyte, if present, causes a substrate having an oxidant cleavable linker and a photosensitizer to come into close proximity. The photosensitizer generates singlet oxygen which oxidatively cleaves the linker to form a product which can be detected in a sandwich detection assay such as LOCI. The amount of product detected is related to the amount of analyte in the medium. Compns., kits, and compds. are also disclosed.

IC ICM C12Q001-68

ICS G01N033-53

INCL 435006000; 435007100

CC 9-10 (Biochemical Methods)

Section cross-reference(s): 3, 10, 14

ST amplified luminescent homogeneous immunoassay

IT Immunoassay

(Amplified luminescent homogeneous; amplified luminescent homogeneous immunoassay)

IT Analysis

(Binding; amplified luminescent homogeneous immunoassay)

IT Immunoassay

(Enhanced Loci Homogeneous; amplified luminescent homogeneous immunoassay)

IT Immunoassay

(Fluorescent oxygen channeling assay; amplified luminescent homogeneous immunoassay)

IT Linking agents

(Oxidant cleavable; amplified luminescent homogeneous immunoassay)

IT Molecules

(enol, thio containing; amplified luminescent homogeneous immunoassay)

IT Ethers, uses  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (enol; amplified luminescent homogeneous immunoassay)

IT Immunoassay  
 (enzyme-linked immunosorbent assay; amplified luminescent homogeneous immunoassay)

IT Immunoassay  
 (fluorescence energy transfer; amplified luminescent homogeneous immunoassay)

IT Antigens  
 RL: ANT (Analyte); ANST (Analytical study)  
 (hepatitis B surface; amplified luminescent homogeneous immunoassay)

IT Immunoassay  
 (luminescent oxygen channeling; amplified luminescent homogeneous immunoassay)

IT Antibodies and Immunoglobulins  
 RL: ANT (Analyte); ANST (Analytical study)  
 (monoclonal; amplified luminescent homogeneous immunoassay)

IT Group IIIA element compounds  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (organometallic compds.; amplified luminescent homogeneous immunoassay)

IT Bond cleavage  
 (oxidative; amplified luminescent homogeneous immunoassay)

IT 91-20-3D, Naphthalene, derivs. 101-80-4, p-Aminophenyl ether.  
 120-12-7D, Anthracene, derivs. 288-32-4D, Imidazole, derivs.  
 288-42-6D, Oxazole, derivs. 288-47-1D, Thiazole, derivs. 302-01-2D,  
 Hydrazine, diacyl derivs. 543-75-9D, Dioxene, derivs. 1965-09-9,  
 p-Hydroxyphenyl ether 6538-93-8D, derivs. 23230-01-5D, derivs.  
 648425-48-3D, derivs. 753001-07-9 753001-08-0 753001-09-1  
 753001-11-5  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (amplified luminescent homogeneous immunoassay)

IT 753000-99-6DP, beads coated with, conjugated with nucleotides  
 753001-04-6P  
 RL: ARG (Analytical reagent use); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (amplified luminescent homogeneous immunoassay)

IT 753001-12-6P  
 RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)  
 (amplified luminescent homogeneous immunoassay)

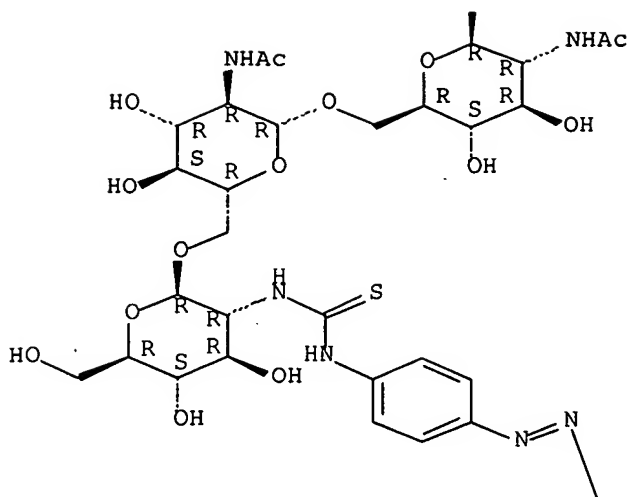
IT 7722-84-1, Hydrogen peroxide, formation (nonpreparative)  
 RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)  
 (amplified luminescent homogeneous immunoassay)

IT 79-37-8, Oxalyl chloride 98-59-9, Tosyl chloride 100-52-7,  
 Benzaldehyde, reactions 100-61-8, reactions 107-15-3,  
 1,2-Diaminoethane, reactions 121-44-8, Triethylamine, reactions  
 429-41-4, Tetrabutylammonium fluoride 1075-06-5, Phenyl glyoxal  
 monohydrate 1672-46-4 2365-48-2, Methyl thioglycolate 7440-23-5,  
 Sodium metal, reactions 9004-54-0, Dextran T-500, reactions  
 9004-54-0D, Dextran, aldehyde derivs. 9013-20-1, Streptavidin  
 10026-04-7, Silicon tetrachloride 14660-52-7, Ethyl 5-bromovalerate  
 14794-31-1, Ethyl succinyl chloride 25895-60-7, Sodium cyano borohydride  
 29797-09-9, Cyclohexadiene 32703-80-3, 4-tert-Butyl-1,2-dicyanobenzene  
 90867-06-4 100023-76-5 134759-23-2, Siac 206557-09-7, 2-Amino 9,10

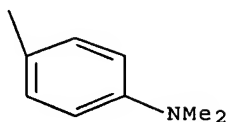
Two mols., a fluorophore (5-(2-aminoethyl) amino-1-naphthalene-sulfonic acid; EDANS) and a quenching group (dimethylaminophenylazophenyl; DAB) were chemical introduced on to the chitopentaose, one at each end. Among eight enzymes tested, only endo-chitinase and chitobiosidase activities could be specifically assayed by monitoring the variation of fluorescence after enzymic hydrolysis of this substrate. Chitobioses and N-acetyl- $\beta$ -glucosaminidases are not active on the compound, the presence of a bulky chromogenic group at the 2 position of the nonreducing end of the substrate preventing the binding and thus hydrolysis by these two exo-enzymes. The observation that chitobiosidases are able to hydrolyze a chitooligosaccharide functionalized on both extremities demonstrates the possibility of an endo-action for this class of chitinases, which are generally classified as exo-enzymes. This fluorogenic chitooligosaccharide should prove to be very useful for the detection and the convenient assay of chitinolytic activities at nanomolar concns.

- CC 7-1 (Enzymes)  
Section cross-reference(s): 33
- ST chitopentaose substrate endochitinase chitobiosidase detn  
fluorescence; chitinase detn chitopentaose substrate  
fluorescence
- IT Enzyme kinetics  
Michaelis constant  
(a fluorescence-quenched chitopentaose for the study of  
endo-chitinases and chitobiosidases)
- IT 9001-06-3, Endo-chitinase 9001-63-2, Lysozyme 146702-78-5,  
exo-N,N1-Diacetylchiobiohydrolase  
RL: ANT (Analyte); BAC (Biological activity or effector, except adverse);  
BSU (Biological study, unclassified); ANST (Analytical study); BIOL  
(Biological study)  
(a fluorescence-quenched chitopentaose for the study of  
endo-chitinases and chitobiosidases)
- IT 307299-49-6P  
RL: ARG (Analytical reagent use); BPR (Biological process); BSU  
(Biological study, unclassified); SPN (Synthetic preparation); ANST  
(Analytical study); BIOL (Biological study); PREP (Preparation); PROC  
(Process); USES (Uses)  
(a fluorescence-quenched chitopentaose for the study of  
endo-chitinases and chitobiosidases)
- IT 7612-98-8 71989-18-9 100900-07-0, 5-(2-Aminoethyl)amino-1-naphthalene  
sulfonic acid sodium salt 163777-02-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(a fluorescence-quenched chitopentaose for the study of  
endo-chitinases and chitobiosidases)
- IT 307299-47-4P 307299-48-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(a fluorescence-quenched chitopentaose for the study of  
endo-chitinases and chitobiosidases)
- IT 307299-49-6P  
RL: ARG (Analytical reagent use); BPR (Biological process); BSU  
(Biological study, unclassified); SPN (Synthetic preparation); ANST  
(Analytical study); BIOL (Biological study); PREP (Preparation); PROC  
(Process); USES (Uses)  
(a fluorescence-quenched chitopentaose for the study of  
endo-chitinases and chitobiosidases)
- RN 307299-49-6 HCAPLUS
- CN 1-Naphthalenesulfonic acid, 5-[[[2-[[[(2R)-1-[O-2-deoxy-2-[[[4-[[4-  
(dimethylamino)phenyl]azo]phenyl]amino]thioxomethyl]amino]- $\beta$ -D-  
glucopyranosyl-(1 $\rightarrow$ 6)-O-2-(acetylamino)-2-deoxy- $\beta$ -D-

PAGE 2-A



PAGE 3-A



IT 307299-48-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (a fluorescence-quenched chitopentaose for the study of  
 endo-chitinases and chitobiosidases)

RN 307299-48-5 HCAPLUS

CN 1-Naphthalenesulfonic acid, 5-[[2-[[[(2R)-1-[O-2-amino-2-deoxy-β-D-  
 glucopyranosyl-(1→6)-O-2-(acetylamino)-2-deoxy-β-D-  
 glucopyranosyl-(1→6)-O-2-(acetylamino)-2-deoxy-β-D-  
 glucopyranosyl-(1→6)-O-2-(acetylamino)-2-deoxy-β-D-  
 glucopyranosyl-(1→6)-2-(acetylamino)-2-deoxy-β-D-  
 glucopyranosyl]-5-oxo-2-pyrrolidiny]carbonyl]amino]ethyl]amino] - (CA  
 INDEX NAME)

Absolute stereochemistry.

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L165 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:62989 HCAPLUS Full-text

DOCUMENT NUMBER: 128:177815

TITLE: A quenching fluoroimmunoassay for analysis of the pesticide propazine in an apolar organic solvent, reverse micelles of AOT in n-octane: effect of the micellar matrix and labeled antigen structure

AUTHOR(S): Matveeva, E. G.; Samsonova, J. V.; Eremin, S. A.

CORPORATE SOURCE: A.N. Bakh Inst. Biochem., Russian Academy Sci., Moscow, 117071, Russia

SOURCE: Journal of Fluorescence (1997), 7(3), 211-216

CODEN: JOFLEN; ISSN: 1053-0509

PUBLISHER: Plenum Publishing Corp.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A simple way of directly observing antigen-antibody binding in a reverse micellar system, n-octane containing reverse micelles of aerosol OT (AOT), using the hydrophobic pesticide propazine as antigen, is described. We observed two processes during fluorescein-labeled propazine (FP)-antibody (Ab) interaction in reverse micelles: (1) quenching of the fluorescence of FP after mixing of Ab and FP (due immune complex formation) and (2) restoration of FP fluorescence after addition of excess propazine to the immune complex formed. We found that the quenching efficiency depends on both the properties of the reverse micellar system (surfactant concentration, hydration degree  $W_0 = [\text{water}]/[\text{surfactant}]$ ) and the structure of the labeled antigen. A quenching fluoroimmunoassay of propazine both in apolar organic solvents and in water is developed. The method is homogeneous. The quenching time is 10-30 min, and the detection limit of propazine is 100 nM (20 µg/L) in organic solvent and 10 nM (2 µg/L) in water. Propazine can be added to the reverse micellar system when dissolved in AOT/octane, or in an octane/chloroform mixture, or in chloroform. This makes possible the use of the anal. directly for pesticide exts. in nonpolar-organic solvents.

CC 9-10 (Biochemical Methods)

Section cross-reference(s): 5, 6

ST propazine quenching fluoroimmunoassay reversed micelle

IT Immunoassay

(fluorescence, quenching; quenching fluoroimmunoassay for anal. of the pesticide propazine in an apolar organic solvent, reverse micelles of AOT in n-octane)

IT Fluorescence quenching

Molecular association

(quenching fluoroimmunoassay for anal. of the pesticide propazine in an apolar organic solvent, reverse micelles of AOT in n-octane)

IT Antibodies

Antigens

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(quenching fluoroimmunoassay for anal. of the pesticide propazine in an apolar organic solvent, reverse micelles of AOT in n-octane)

IT Micelles

(reverse; quenching fluoroimmunoassay for anal. of the pesticide propazine in an apolar organic solvent, reverse micelles of AOT in n-octane)

IT 139-40-2, Propazine

RL: ANT (Analyte); BPR (Biological process); BSU (Biological study,

TITLE: Compositions and methods for use in detection of analytes  
 INVENTOR(S): Reddy, M. Parameswara; Sternberg, James C.  
 PATENT ASSIGNEE(S): Beckman Instruments, Inc., USA  
 SOURCE: PCT Int. Appl., 59 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9606948	A1	19960307	WO 1995-US10226	19950810 <--
W: AU, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 5648213	A	19970715	US 1994-298523	19940830 <--
AU 9532431	A	19960322	AU 1995-32431	19950810 <--
AU 698206	B2	19981029		
EP 779934	A1	19970625	EP 1995-928819	19950810 <--
EP 779934	B1	20000405		
R: DE, ES, FR, GB, IT				
JP 10504962	T	19980519	JP 1996-508779	19950810 <--
JP 3520298	B2	20040419		

PRIORITY APPLN. INFO.:  
 US 1994-298523 A 19940830 <--  
 WO 1995-US10226 W 19950810 <--

AB Double-stranded nucleic acid duplexes serve as universal harvestable and cleavable link systems in a variety of different types of immunoassays (e.g., sandwich, competitive, etc.). Depending upon the type of assay, at least one specific component involved in the assay system is attached to a first member of a pair of sequences forming a double-stranded nucleic acid (i.e., two oligonucleotides comprising substantially complementary sequences). The assay is carried out in the presence of a support to which is attached an oligonucleotide which is the other member of the pair of sequences forming a double-stranded nucleic acid duplex under hybridization conditions. Upon the hybridization of the two complementary oligonucleotides to form a duplex, the component of the assay system to which the first member of the pair of oligonucleotides is attached may thereby be effectively removed from the solution phase and harvested onto the support. Oligonucleotides bound to a support are reusable in multiple successive assays. Moreover, any given support-bound oligonucleotide can be used in accordance with the present invention for the anal. of a variety of different analytes. In many cases, the assay system includes a label to facilitate quantifying the amount of analyte; in others, the amount of analyte may be determined without the use of any extraneous label. Examples show the determination of phenobarbital, theophylline, and TSH and combinations of 2 or all 3 of them.

IC ICM C12Q001-68  
 ICS G01N021-64

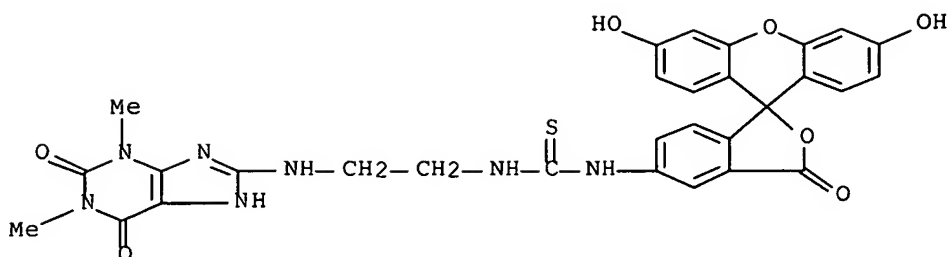
CC 9-10 (Biochemical Methods)  
 Section cross-reference(s): 1, 2, 3, 15

ST immunoassay double stranded nucleic acid hybridization; drug  
 detn immunoassay nucleic acid hybridization; hormone detn  
 immunoassay nucleic acid hybridization

IT Fluorescent substances  
 Immobilization

Immunoassay  
 Nucleic acid hybridization  
 Optical fibers

(double-stranded nucleic acids as universal link system in immunoassays)



L165 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:562386 HCAPLUS Full-text

DOCUMENT NUMBER: 122:322049

TITLE: Fluorescence-polarization

immunoassay for sym-1,3,5-triazine herbicides

AUTHOR(S): Samsonova, Zh. V.; Eremin, S. A.; Egorov, A. M.

CORPORATE SOURCE: M. V. Lomonosov, Moscow State Univ., Moscow, Russia

SOURCE: Voprosy Meditsinskoi Khimii (1994), 40(4),

53-6

CODEN: VMDKAM; ISSN: 0042-8809

PUBLISHER: Meditsina

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB The sensitivity of a fluorescence-polarization immunoassay with fluorescein-labeled atrazine derivs. can be increased by shortening the length of the chemical bridge between the antigen and the fluorescent label. The detection limit for atrazine in a 50  $\mu$ L sample was 6 ng/mL. The total time required for processing 10 samples was approx. 7 min. The method may be used for environmental monitoring of sym-triazine herbicides in water samples.

CC 61-3 (Water)

Section cross-reference(s): 5

ST immunoassay fluorescence polarization triazine herbicide

IT Herbicides

(atrazine; fluorescence-polarization immunoassay)

IT Immunoassay

(fluorescence-polarization, for triazine herbicides)

IT 7732-18-5, Water, analysis

RL: AMX (Analytical matrix); ANST (Analytical study)  
(fluorescence-polarization immunoassay for triazine herbicides)

IT 139-40-2, Propazine 834-12-8, Ametryn 1912-24-9, Atrazine 7287-19-6, Prometryn

RL: ANT (Analyte); ANST (Analytical study)  
(fluorescence-polarization immunoassay for triazine herbicides)

IT 163405-32-1P 163405-33-2P 163405-34-3P

RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)  
(fluorescence-polarization immunoassay for triazine herbicides)

IT 163405-32-1P

RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)  
(fluorescence-polarization immunoassay for triazine herbicides)

RN 163405-32-1 HCAPLUS

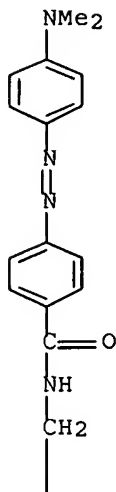


(fluorescence of)

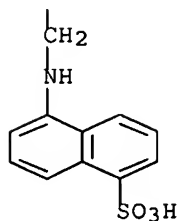
RN 131941-78-1 HCAPLUS

CN 1-Naphthalenesulfonic acid, 5-[[2-[[4-[[4-(dimethylamino)phenyl]azo]benzoyl]amino]ethyl]amino]- (9CI) (CA INDEX NAME)

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PAGE 2-A



L165 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1989:91693 HCAPLUS Full-text

DOCUMENT NUMBER: 110:91693

TITLE: Benzodiazepines assay, tracers, immunogens and antibodies

INVENTOR(S): Wang, Nai Yi; Keegan, Candace Linda; Heiman, Daniel Fuelner; Flentge, Charles Arthur; Wang, Philip Pei

PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: Eur. Pat. Appl., 25 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

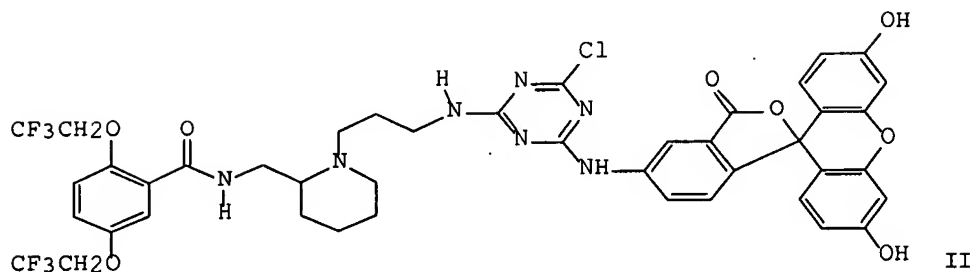
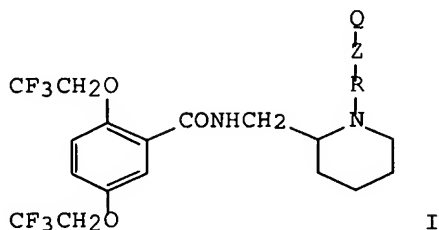
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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- (to benzodiazepines, for fluorescence-polarization immunoassay)
- IT Albumins, compounds  
RL: ANST (Analytical study)  
(conjugates, with benzodiazepine derivs., as immunogens for fluorescence-polarization immunoassay)
- IT Amino acids, polymers  
RL: ANST (Analytical study)  
(polymers, conjugates, with benzodiazepine derivs., as immunogens for fluorescence-polarization immunoassay)
- IT 75-44-5, Phosgene 463-71-8, Thiophosgene 538-75-0,  
N,N'-Dicyclohexylcarbodiimide 1892-57-5 15580-20-8  
RL: ANST (Analytical study)  
(as coupling agent in preparation of immunogen for fluorescence-polarization immunoassay for benzodiazepines)
- IT 12794-10-4D, Benzodiazepine, derivs.  
RL: ANT (Analyte); ANST (Analytical study)  
(determination of, by fluorescence-polarization immunoassay, synthesis of immunogens and tracers for)
- IT 1088-11-5P 27016-88-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, in synthesis of immunogens for fluorescence-polarization immunoassay for benzodiazepines)
- IT 119194-45-5P 119194-51-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, in synthesis of precursor for immunogen or tracer for fluorescence-polarization immunoassay for benzodiazepines)
- IT 119194-47-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, in synthesis of tracer for fluorescence-polarization immunoassay for benzodiazepines)
- IT 4959-16-4DP, albumin conjugates 27016-88-2DP, albumin conjugates  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as immunogen for fluorescence-polarization immunoassay for benzodiazepines)
- IT 119194-49-9P 119194-50-2P 119194-52-4P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as precursor for immunogen or tracer for fluorescence-polarization immunoassay for benzodiazepines)
- IT 119194-48-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as precursor for tracer for fluorescence-polarization immunoassay for benzodiazepines)
- IT 119194-41-1P 119194-42-2P 119194-44-4P 119194-46-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as tracer for fluorescence-polarization immunoassay for benzodiazepines)
- IT 2321-07-5DP, Fluorescein, benzodiazepine derivative conjugates 3301-79-9DP, benzodiazepine derivative conjugates 3326-34-9DP, benzodiazepine derivative conjugates 51649-83-3DP, benzodiazepine derivative conjugates 76823-03-5DP, benzodiazepine derivative conjugates 119194-53-5DP, benzodiazepine derivative conjugates 119194-54-6DP, benzodiazepine derivative

CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 242847	A2	19871028	EP 1987-105832	19870421 <--
EP 242847	A3	19890222		
EP 242847	B1	19930602		
R: BE, DE, FR, IT				
JP 62267289	A	19871119	JP 1987-100174	19870424 <--
CA 1321998	C	19930907	CA 1987-535491	19870424 <--
US 5336622	A	19940809	US 1989-336574	19890411 <--
PRIORITY APPLN. INFO.:			US 1986-856079	A 19860425 <--
			US 1987-132083	B1 19871211 <--

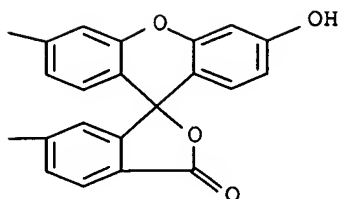
GI



AB Flecainide is determined in fluids, especially biol. fluids such as serum, plasma, or urine, by a fluorescence polarization immunoassay using tracer I (R = linking group of ≤10 hetero atoms and a total of 0-20 C and hetero atoms in a straight or branched chain containing ≤2 rings; Z = NH, C:O, SO<sub>2</sub>, C:NH; Q = fluorescein or derivative thereof) prepared by coupling fluorescein or its derivative to tracer precursor I (R as above; Z = NH, S, O, C:O, SO<sub>2</sub>, C:NH; Q = H, OH, leaving group). N-(3-Aminopropyl)flecainide was reacted with 2-(fluorescein-5-ylamino)-4,6-dichloro-1,3,5-triazine at ambient temperature in MeOH for 24 h. Tracer II was purified by chromatog. on silica gel thin-layer plates with CHCl<sub>3</sub>-MeOH and C<sub>6</sub>H<sub>6</sub>-AcOEt-Me<sub>2</sub>CO.

IC ICM C07D251-50  
 ICS C07D211-00; G01N033-49; G01N033-58; G01N021-64  
 ICA G01N033-94; G01N033-533  
 CC 1-1 (Pharmacology)  
 Section cross-reference(s): 27  
 ST flecainide fluorescence polarization immunoassay

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L165 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1984:206160 HCAPLUS Full-text  
 DOCUMENT NUMBER: 100:206160  
 ORIGINAL REFERENCE NO.: 100:31253a,31256a  
 TITLE: Fluorescent polarization immunoassay  
 utilizing substituted triazinylaminofluoresceins  
 INVENTOR(S): Wang, Chao Huei J.; Stroupe, Stephen D.; Jolley,  
 Michael E.  
 PATENT ASSIGNEE(S): Abbott Laboratories, USA  
 SOURCE: U.S., 13 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 6  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4420568	A	19831213	US 1981-325872	19811130 <--
CA 1160626	A1	19840117	CA 1981-379747	19810615 <--
GB 2081257	A	19820217	GB 1981-18754	19810618 <--
GB 2081257	B	19841107		
AU 8172036	A	19820204	AU 1981-72036	19810622 <--
AU 554360	B2	19860821		
SE 8104227	A	19820131	SE 1981-4227	19810707 <--
DE 3129705	A1	19820527	DE 1981-3129705	19810728 <--
DE 3129705	C2	19880310		
BE 889788	A1	19820129	BE 1981-205525	19810729 <--
JP 57058695	A	19820408	JP 1981-118573	19810730 <--
US 4492762	A	19850108	US 1982-393577	19820630 <--
US 4593089	A	19860603	US 1983-546778	19831031 <--
US 4420568	B1	19851217	US 1984-90000617	19840824 <--
US 4492762	B1	19910813	US 1987-90001162	19870206 <--
US 5097097	A	19920317	US 1989-376190	19890630 <--
PRIORITY APPLN. INFO.:			US 1980-173553	A2 19800730 <--
			US 1981-235259	A2 19810217 <--
			US 1981-325872	A2 19811130 <--
			US 1981-329974	A2 19811211 <--
			US 1981-329975	A2 19811211 <--
			US 1982-393577	A 19820630 <--
			US 1983-546778	B3 19831031 <--
			US 1986-865992	B1 19860522 <--
			US 1987-90001314	A 19870825 <--

90275-51-7P 90275-52-8P 90275-53-9P 90275-54-0P 90275-55-1P  
 90275-56-2P 90275-57-3P 90275-58-4P 90275-59-5P 90275-60-8P  
 90275-61-9P 90275-62-0P 90275-63-1P 90275-64-2P 90275-65-3P  
 90275-66-4P 90296-63-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

IT 82169-58-2 90275-37-9

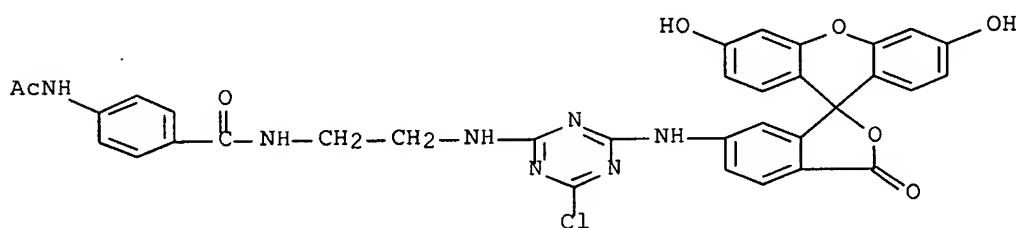
RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with desethylacetylprocainamide)

IT 90275-38-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 90275-38-0 HCAPLUS

CN Benzamide, 4-(acetylamino)-N-[2-[[4-chloro-6-[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl)amino]-1,3,5-triazin-2-yl]amino]ethyl]- (CA INDEX NAME)

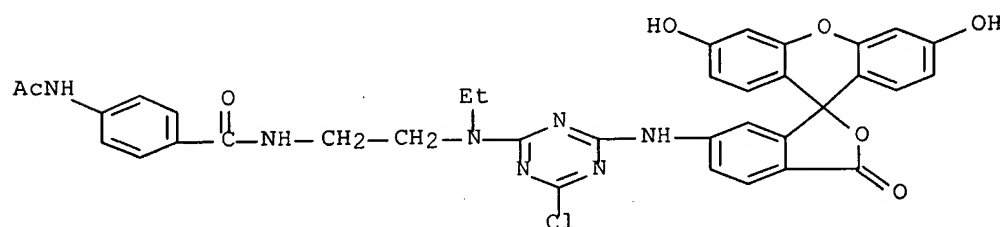


IT 90275-37-9

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with desethylacetylprocainamide)

RN 90275-37-9 HCAPLUS

CN Benzamide, 4-(acetylamino)-N-[2-[[4-chloro-6-[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl)amino]-1,3,5-triazin-2-yl]ethylamino]ethyl]- (CA INDEX NAME)



OR L90))

L94 1407 SEA FILE=HCAPLUS ABB=ON L93

L122 573 SEA FILE=HCAPLUS ABB=ON L94 (L) (THU OR BAC OR PAC OR PKT OR DMA)/RL

L130 912 SEA FILE=HCAPLUS ABB=ON L94 AND (PY<2001 OR AY<2001 OR PRY<2001)

L150 90112 SEA FILE=HCAPLUS ABB=ON KI/BI

L158 13 SEA FILE=HCAPLUS ABB=ON L130 AND L150 AND L122

=> s l160,l157,l158 not l96,l163,l164,l165

L167 21 (L160 OR L157 OR L158) NOT (L96 OR L163 OR L164 OR L165)

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L167 ANSWER 1 OF 21 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:316276 HCAPLUS Full-text

DOCUMENT NUMBER: 142:392424

TITLE: Preparation of aminopyrrolopyrimidines as adenosine A1 receptor antagonists.

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan; Witter, David J.

PATENT ASSIGNEE(S): OSI Pharmaceuticals, Inc., USA

SOURCE: U.S., 66 pp., Cont.-in-part of Appl. No.

PCT/US99/12135.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6878716	B1	20050412	US 1999-454074	19991202 <--
WO 9962518	A1	19991209	WO 1999-US12135	19990601 <--
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 443760-78-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);  
 THU (Therapeutic use); BIOL (Biological study); PREP  
 (Preparation); USES (Uses)

(preparation of aminopyrrolopyrimidines as adenosine A1 receptor  
 antagonists)

IT 251946-03-9 251947-22-5 251947-24-7 343631-98-1 343632-04-2  
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 343632-12-2 343632-13-3 343632-14-4 343632-15-5  
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RL: PAC (Pharmacological activity); THU (Therapeutic  
 use); BIOL (Biological study); USES (Uses)

(preparation of aminopyrrolopyrimidines as adenosine A1 receptor  
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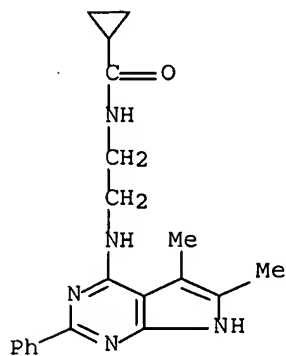
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation);  
 THU (Therapeutic use); BIOL (Biological study); PREP  
 (Preparation); USES (Uses)

(preparation of aminopyrrolopyrimidines as adenosine A1 receptor  
 antagonists)

RN 251946-27-7 HCAPLUS

CN Cyclopropanecarboxamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-  
 d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)



RN 443760-78-9 HCAPLUS

CN Cyclopropanecarboxamide, 1-amino-N-[2-[(2-phenyl-1H-pyrrolo[2,3-  
 d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

FAMILY ACC. NUM. COUNT: 4

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6686366	B1	20040203	US 1999-454075	19991202 <--
WO 9962518	A1	19991209	WO 1999-US12135	19990601 <--
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WO 2001039777	A1	20010607	WO 2000-US32702	20001201 <--
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HK 1050319	A1	20070404	HK 2003-102257	20030328 <--
PRIORITY APPLN. INFO.:				
			US 1998-87702P	P 19980602 <--
			US 1999-123216P	P 19990308 <--
			US 1999-126527P	P 19990326 <--
			WO 1999-US12135	A2 19990601 <--
			US 1999-454074	A 19991202 <--
			US 1999-454075	A 19991202 <--
			US 1999-454254	A 19991202 <--
			EP 2000-988011	A3 20001201 <--
			WO 2000-US32702	W 20001201 <--

OTHER SOURCE(S): MARPAT 140:146159

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 653600-36-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);  
 THU (Therapeutic use); BIOL (Biological study); PREP  
 (Preparation); USES (Uses)

(preparation and use of substituted 7H-pyrrolo[2,3-d]pyrimidines as  
 selective adenosine A3 receptor antagonists)

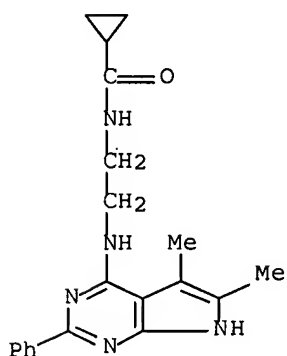
IT 251946-27-7P 343631-99-2P 343632-15-5P  
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation);  
 THU (Therapeutic use); BIOL (Biological study); PREP  
 (Preparation); USES (Uses)

(preparation and use of substituted 7H-pyrrolo[2,3-d]pyrimidines as  
 selective adenosine A3 receptor antagonists)

RN 251946-27-7 HCAPLUS

CN Cyclopropanecarboxamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-  
 d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)



RN 343631-99-2 HCAPLUS

CN Acetamide, 2-(cyclopropylamino)-N-[2-[(5,6-dimethyl-2-phenyl-1H-  
 pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 128 THERE ARE 128 CITED REFERENCES AVAILABLE FOR  
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT

L167 ANSWER 3 OF 21 HCAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2002:72050 HCAPLUS Full-text  
DOCUMENT NUMBER: 136:118449  
TITLE: Preparation of heterocyclic beta-3 adrenergic receptor  
agonists  
INVENTOR(S): Ashwell, Mark Anthony; Solvibile, William Ronald  
PATENT ASSIGNEE(S): American Home Products Corporation, USA  
SOURCE: PCT Int. Appl., 64 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002006235	A1	20020124	WO 2001-US22366	20010716 <--
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US 2002022638	A1	20020221	US 2001-904115	20010712 <--
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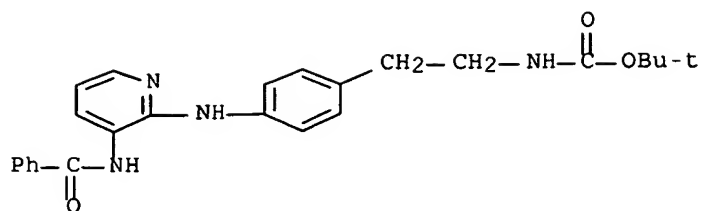
PRIORITY APPLN. INFO.: US 2000-218700P P 20000717 <--

AB This invention provides A-U-CH(OH)CH<sub>2</sub>NHCH<sub>2</sub>CH<sub>2</sub>VC<sub>6</sub>H<sub>4</sub>W-p (1) or a pharmaceutically acceptable salt thereof, which are useful in treating or inhibiting metabolic disorders related to insulin resistance or hyperglycemia (typically associated with obesity or glucose intolerance), atherosclerosis, gastrointestinal disorders, neurogenic inflammation, glaucoma, ocular hypertension and frequent urination; and are particularly useful in the treatment or inhibition of type II diabetes.  $\beta$ 3-Adrenergic receptor EC<sub>50</sub> and maximal response (IA; % activity compound/% activity isoproterenol) values are reported for 16 example compds., e.g. 0.057  $\mu$ M and 1.12 for 3-[4-[2-[(2S)-2-hydroxy-3-(4-hydroxyphenoxy)propylamino]ethyl]phenyl]-1-isopropenyl-1,3-dihydroimidazo[4,5-b]pyridin-2-one. In 1, A is (a) a 5-6 membered heterocyclic ring having 1-4 heteroatoms selected from O, N, and S, substituted with (R<sub>1</sub>)m; (b) a Ph ring substituted with (R<sub>1</sub>)m; (c) a naphthyl ring substituted with (R<sub>1</sub>)m; or (d) a Ph fused heterocycle selected from (R<sub>1</sub>)m-substituted 1,3-dihydro-2-oxo-2H-benzimidazol-4-yl, 1,3-benzodioxol-5-yl, 1,2,3,4-tetrahydro-2-oxoquinolin-5-yl, 1,2,3,4-tetrahydro-1-naphthylideneamino. U is -OCH<sub>2</sub>- or a bond; V is O or a bond; W is an amino or amido group wherein the N is substituted by an optionally substituted pyridyl or pyrazinyl ring or the N is incorporated into an imidazole ring fused with a pyridine or pyrazine ring. R<sub>1</sub> is alkyl of 1-8 C atoms, aryl of 6-10 C atoms, -OR<sub>7</sub>, cycloalkyl of 3-8 C atoms, halogen, cyano, trifluoromethyl, CO<sub>2</sub>R<sub>7</sub>, NHCOR<sub>7</sub>, NH<sub>2</sub>SO<sub>2</sub>R<sub>7</sub>, -NR<sub>7</sub>CONR<sub>8</sub>R<sub>9</sub>, -NR<sub>7</sub>R<sub>8</sub>, alkenyl of 2-7 C atoms, S(O)<sub>v</sub>R<sub>7</sub>, NO<sub>2</sub>, -O(CH<sub>2</sub>)<sub>u</sub>CO<sub>2</sub>R<sub>7</sub>, -OCONR<sub>7</sub>R<sub>8</sub>, -O(CH<sub>2</sub>)<sub>s</sub>OR<sub>7</sub>, or a 5-6 membered heterocyclic ring containing 1 to 4 heteroatoms selected from O, S, and N. R<sub>2</sub>, R<sub>4</sub>, R<sub>7</sub>, R<sub>8</sub>, and R<sub>9</sub> are each, independently, H, alkyl of 1-8 C atoms, aryl of 6-10 C atoms,

isopropenyl-1,3-dihydro-2H-imidazo[4,5-b]pyridin-2-one 391674-22-9P,  
 tert-Butyl 4-[2-(4-ethylphenyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenethylcarbamate 391674-24-1P, 2-[4-[2-(4-Ethylphenyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenyl]-1-ethanamine formate 391674-25-2P,  
 (2S)-1-[4-[(tert-Butyldiphenylsilyl)oxy]phenoxy]-3-[[4-[2-(4-ethylphenyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenethyl]amino]-2-propanol 391674-27-4P,  
 tert-Butyl 4-(2-pentyl-3H-imidazo[4,5-b]pyridin-3-yl)phenethylcarbamate 391674-28-5P, (2S)-1-[4-[(tert-Butyldiphenylsilyl)oxy]phenoxy]-3-[[4-(2-pentyl-3H-imidazo[4,5-b]pyridin-3-yl)phenethyl]amino]-2-propanol 391674-30-9P, tert-Butyl 4-[2-(4-cyclohexylphenyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenethylcarbamate 391674-31-0P, 4-[2-(4-Cyclohexylphenyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenethylamine 391674-32-1P, (2S)-1-[4-[(tert-Butyldiphenylsilyl)oxy]phenoxy]-3-[[4-[2-(4-cyclohexylphenyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenethyl]amino]-2-propanol 391674-34-3P, tert-Butyl 4-[2-(2-cyclopentylethyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenethylcarbamate 391674-35-4P, 4-[2-(2-Cyclopentylethyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenethylamine 391674-36-5P, (2S)-1-[4-[(tert-Butyldiphenylsilyl)oxy]phenoxy]-3-[[4-[2-(2-cyclopentylethyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenethyl]amino]-2-propanol 391674-40-1P, tert-Butyl 4-[2-[2-chloro-4-(3-methyl-1H-pyrazol-1-yl)phenyl]-3H-imidazo[4,5-b]pyridin-3-yl]phenethylcarbamate 391674-42-3P, 2-[4-[2-[2-Chloro-4-(3-methyl-1H-pyrazol-1-yl)phenyl]-3H-imidazo[4,5-b]pyridin-3-yl]phenyl]-1-ethanamine formate 391674-43-4P, (2S)-1-[4-[(tert-Butyldiphenylsilyl)oxy]phenoxy]-3-[[4-[2-[2-chloro-4-(3-methyl-1H-pyrazol-1-yl)phenyl]-3H-imidazo[4,5-b]pyridin-3-yl]phenethyl]amino]-2-propanol 391674-44-5P, N-(4-Cyanophenyl)-N'-hexylurea 391674-45-6P, Methyl 4-[[[(hexylamino)carbonyl]amino]benzenecarboximidate 391674-46-7P, tert-Butyl 4-[2-[4-[[[(hexylamino)carbonyl]amino]phenyl]-3H-imidazo[4,5-b]pyridin-3-yl]phenethylcarbamate 391674-48-9P, N-[4-[3-[4-(2-Aminoethyl)phenyl]-3H-imidazo[4,5-b]pyridin-2-yl]phenyl]-N'-hexylurea formate 391674-49-0P, N-[4-[3-[4-[2-[[[(2S)-3-[4-[(tert-Butyldiphenylsilyl)oxy]phenoxy]-2-hydroxypropyl]amino]ethyl]phenyl]-3H-imidazo[4,5-b]pyridin-2-yl]phenyl]-N'-hexylurea 391674-52-5P, Methyl 4-[[[(hexylamino)carbonyl]amino]benzoate 391674-53-6P, 4-[[[(Hexylamino)carbonyl]amino]benzoic acid 391674-54-7P, tert-Butyl 4-[2-[3-[[[(hexylamino)carbonyl]amino]phenyl]-3H-imidazo[4,5-b]pyridin-3-yl]phenethylcarbamate 391674-57-0P, N-[3-[3-[4-(2-Aminoethyl)phenyl]-3H-imidazo[4,5-b]pyridin-2-yl]phenyl]-N'-hexylurea formate 391674-58-1P, N-[3-[3-[4-[2-[[[(2S)-3-[4-[(tert-Butyldiphenylsilyl)oxy]phenoxy]-2-hydroxypropyl]amino]ethyl]phenyl]-3H-imidazo[4,5-b]pyridin-2-yl]phenyl]-N'-hexylurea 391674-60-5P, tert-Butyl 4-[2-[4-[[[(hexylamino)carbonyl]amino]phenethyl]-3H-imidazo[4,5-b]pyridin-3-yl]phenethylcarbamate 391674-63-8P, N-[4-[2-[3-[4-(2-Aminoethyl)phenyl]-3H-imidazo[4,5-b]pyridin-2-yl]ethyl]phenyl]-N'-hexylurea formate 391674-64-9P, N-[4-[2-[3-[4-[2-[[[(2S)-3-[4-[(tert-Butyldiphenylsilyl)oxy]phenoxy]-2-hydroxypropyl]amino]ethyl]phenyl]-3H-imidazo[4,5-b]pyridin-2-yl]ethyl]phenyl]-N'-hexylurea  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

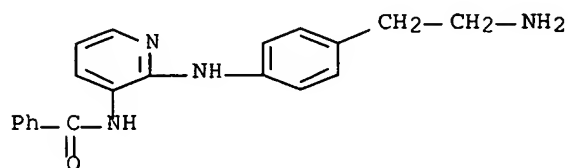
(intermediate; preparation of heterocyclic amino alc. beta-3 adrenergic receptor agonists)

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RN 391674-14-9 HCAPLUS

CN Benzamide, N-[2-[[4-(2-aminoethyl)phenyl]amino]-3-pyridinyl]- (CA INDEX NAME)

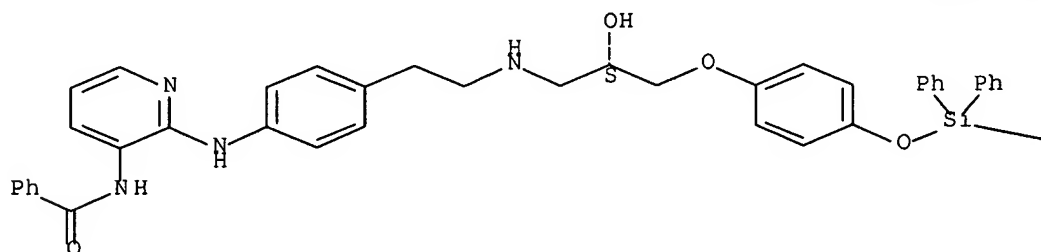


RN 391674-15-0 HCAPLUS

CN Benzamide, N-[2-[[4-[2-[[[(2S)-3-[4-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]phenoxy]-2-hydroxypropyl]amino]ethyl]phenyl]amino]-3-pyridinyl]- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

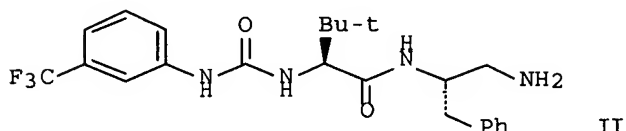
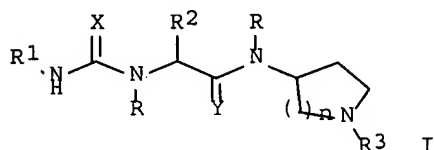


PAGE 1-B

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IT 391674-12-7P, N-[2-[4-[2-[(2S)-2-Hydroxy-3-(4-hydroxyphenoxy)propylamino]ethyl]phenylamino]pyridin-3-yl]benzamide monohydrochloride 391674-69-4P, N-[2-[4-[2-[(2S)-2-Hydroxy-3-(4-hydroxyphenoxy)propylamino]ethyl]phenylamino]pyridin-3-yl]benzamide  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

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 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
 BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
 US 2005080271      A1      20050414      US 2003-203279      20030304 <--  
 US 7115664      B2      20061003  
 US 2007093522      A1      20070426      US 2006-512056      20060829 <--  
 PRIORITY APPLN. INFO.:      US 2000-190133P      P      20000316 <--  
    WO 2001-US6173      W      20010227  
    US 2003-203279      A1      20030304  
 OTHER SOURCE(S):      MARPAT 135:257472  
 GI



AB The invention relates to novel peptidomimetic compds. I [X = O, S; Y = H<sub>2</sub>, O, S; R = H, alkyl, aryl, heteroaryl, aralkyl or heteroaralkyl; R<sub>1</sub>, R<sub>2</sub> = alkyl, aryl, heteroaryl, aralkyl or heteroaralkyl; R<sub>3</sub> = any group given for R or acyl; n = 1, 2 (the stereochem. configuration at any stereocenter may be R,S or a mixture of these configurations)] for use of as ligands, agonists or antagonists, for various cellular receptors, e.g., G-protein-coupled receptors and opioid receptors, and various cellular ion channels, e.g., sodium and calcium. Thus, compound II was prepared by the solid-phase method and showed EC<sub>50</sub> = 0.250 μM opioid agonist activity.

IC ICM C07D207-00

CC 34-3 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 1

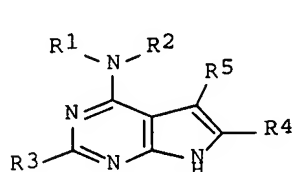
IT 361347-34-4P    361347-36-6P    361347-38-8P    361347-42-4P  
 361347-43-5P    361347-44-6P    361347-45-7P    361347-46-8P    361347-53-7P  
 361347-54-8P    361347-55-9P    361347-56-0P    361347-57-1P    361347-60-6P  
 361347-61-7P    361347-62-8P    361347-63-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

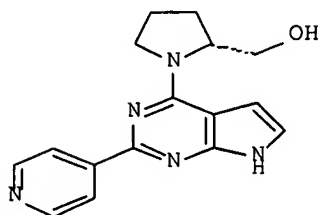
(preparation of peptidomimetic ligands for cellular receptors and ion

DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 4  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001039777	A1	20010607	WO 2000-US32702	20001201 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6686366	B1	20040203	US 1999-454075	19991202 <--
US 6878716	B1	20050412	US 1999-454074	19991202 <--
CA 2393179	A1	20010607	CA 2000-2393179	20001201 <--
EP 1246623	A1	20021009	EP 2000-988011	20001201 <--
EP 1246623	B1	20060809		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003519102	T	20030617	JP 2001-541509	20001201 <--
AU 784878	B2	20060713	AU 2001-24270	20001201 <--
MX 2002PA05357	A	20030519	MX 2002-PA5357	20020529 <--
IN 2002DN00621	A	20070525	IN 2002-DN621	20020619 <--
HK 1050319	A1	20070404	HK 2003-102257	20030328 <--
PRIORITY APPLN. INFO.:				
			US 1999-454074	A 19991202 <--
			US 1999-454075	A 19991202 <--
			US 1999-454254	A 19991202 <--
			US 1998-87702P	P 19980602 <--
			US 1999-123216P	P 19990308 <--
			US 1999-126527P	P 19990326 <--
			WO 1999-US12135	A2 19990601 <--
			WO 2000-US32702	W 20001201 <--
OTHER SOURCE(S): MARPAT 135:46190				
GI				



I



III

AB The synthesis of compds. I, their binding to adenosine receptors and use are described [wherein; R1, R2 = H, (un)substituted alkyl or NR1R2 = (un)substituted 4-8 membered ring; R3 = (un)substituted 4-6 membered (aromatic) ring; R4, R5 = H, (un)substituted alkyl, aryl (with some exceptions)]. Over 100 examples are provided. Intermediate 4-chloro-7H-pyrrolo[2,3-d]pyrimidines were prepared by several routes from appropriately substituted cyano-pyrroles. Thus, 4-chloro-2-(4-pyridyl)-7H-pyrrolo[2,3-

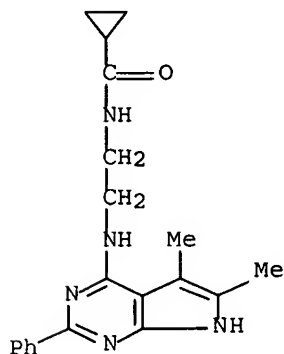
343632-38-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and use of substituted 7H-pyrrolo[2,3-b]pyrimidines as selective adenosine A1, A2a and A3 receptor antagonists)

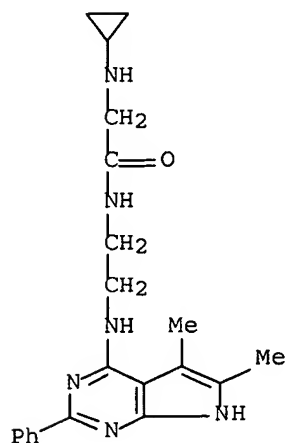
RN 251946-27-7 HCAPLUS

CN Cyclopropanecarboxamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)



RN 343631-99-2 HCAPLUS

CN Acetamide, 2-(cyclopropylamino)-N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)



RN 343632-15-5 HCAPLUS

CN Cyclopropanecarboxamide, 1-amino-N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

WO 9614846                    A1            19960523            WO 1995-US15025            19951116 <--  
 W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI,  
 GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD,  
 MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ,  
 TM, TT  
 RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE,  
 IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR,  
 NE, SN, TD, TG

WO 9717969                    A1            19970522            WO 1996-US18573            19961115 <--  
 W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,  
 DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC,  
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 RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR,  
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 MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

WO 1995-US15025            A2 19951116 <--  
 US 1996-648770            B2 19960516 <--  
 WO 1996-US18573            W 19961115 <--  
 US 1994-340611            A 19941116 <--

OTHER SOURCE(S):            MARPAT 134:340515  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB    Compds. I, II isomers and derivs. are claimed [wherein; M is Ph with up to 5 substituents chosen from H, (branched)(substituted)alkyl, (branched)alk(en)(yn)yl, halo, NO<sub>2</sub>, CN, etc. or two adjacent substituents together constitute a methylenedioxy group; R is H, F, (substituted)alkyl, etc.; R<sub>1</sub> is H, NO<sub>2</sub>, CN, ester, etc.; R<sub>2</sub> is H, (branched)(substituted)alkyl, hydroxyalkyl, alkoxyalkyl, etc.; R<sub>3</sub> is H, (branched)(substituted)alkyl, etc.; Z is alk(en)(yn)yl, CH<sub>2</sub>, O, S(O)<sub>0-2</sub>, CO<sub>2</sub>, amide, urea or (substituted)amino; R<sub>5</sub> and R<sub>6</sub> are H, Cl, Br, I, ester, keto, amide, CN, etc.; R<sub>7</sub> is H, (branched)(substituted)alkyl, hydroxyalkyl, alkoxyalkyl, etc.; n = 0-5; p = 1-7; m = 0-3]. Nineteen example compds. are provided. The synthesis of (+)-III involves a multi-step process utilizing a resolution of a substituted 1-[(4-nitrophenyl)oxycarbonyl]pyrimidine to access an enantiomerically pure pyrimidine which is coupled with the diaminoalkane sidechain. Compds. of the invention are selective antagonists of human  $\alpha$ 1A adrenergic receptors. In competitive binding assays, III had a pK<sub>i</sub> of 5.96, 6.55 and 9.03 for the cloned human  $\alpha$ 1D,  $\alpha$ 1B and  $\alpha$ 1A receptors resp. A 100 mg solid oral dosage formulation (gelatin capsule) was mentioned. Claimed use for invention compds. is treatment of benign prostatic hyperplasia at a dose that is effective but does not cause a fall in blood pressure.

IC    ICM A61K031-505  
 ICS C07D239-22; C07D487-04

INCL 514272000

CC    28-16 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1, 63

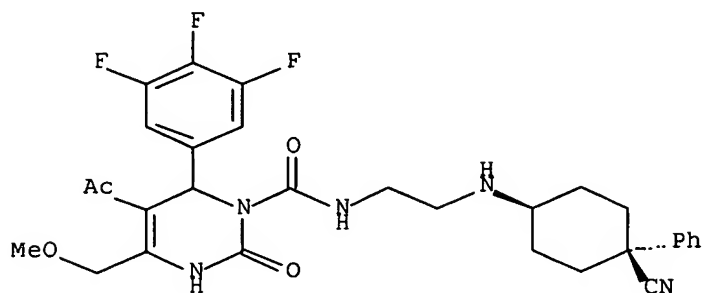
IT    191353-50-1P 191353-51-2P 191353-52-3P  
 191353-53-4P 191353-59-0P 191353-61-4P  
 318236-87-2P 318236-88-3P

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of dihydropyrimidines as selective antagonists for human



trifluorophenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.

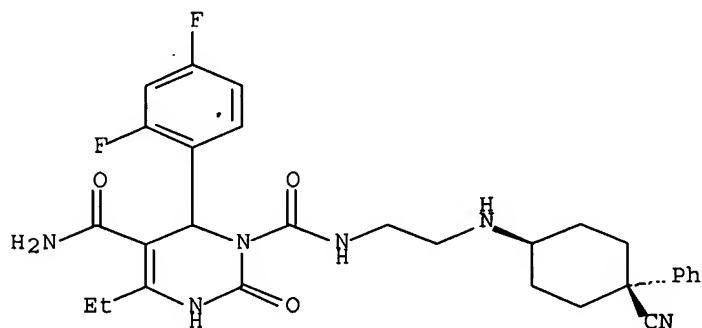


● HCl

RN 191353-51-2 HCAPLUS

CN 1,5(2H)-Pyrimidinedicarboxamide, N1-[2-[(cis-4-cyano-4-phenylcyclohexyl)amino]ethyl]-6-(2,4-difluorophenyl)-4-ethyl-3,6-dihydro-2-oxo-, monohydrochloride, (+)-(9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

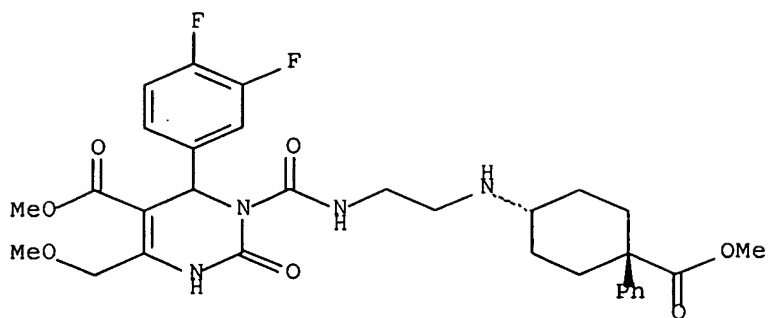


● HCl

RN 191353-52-3 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[(cis-4-cyano-4-phenylcyclohexyl)amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, monohydrochloride, (+)-(9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

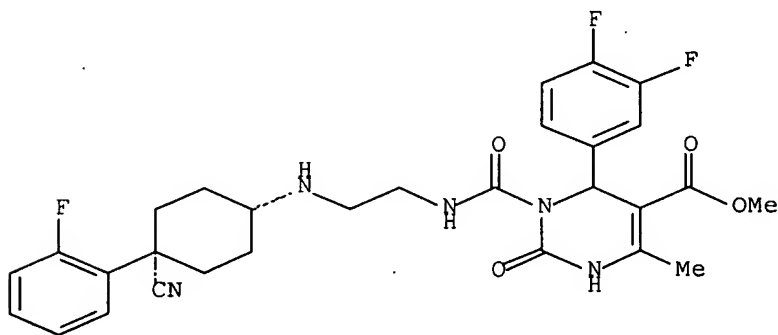


● HCl

RN 191353-61-4 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[[cis-4-cyano-4-(2-fluorophenyl)cyclohexyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-, methyl ester, monohydrochloride, (+)-(9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

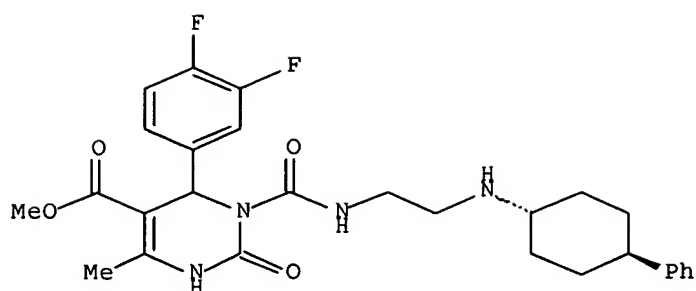


● HCl

RN 318236-87-2 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-1-[[[2-[[[trans-4-(2-pyridinyl)cyclohexyl]amino]ethyl]amino]carbonyl]-, methyl ester, dihydrochloride, (+)-(9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



IT 191353-49-8P 191353-54-5P 191353-56-7P  
 191353-57-8P 191353-58-9P 191353-60-3P  
 191353-67-0P 191353-71-6P 191353-72-7P  
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 318236-93-0P 318236-94-1P 318236-95-2P  
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 318236-99-6P 318237-00-2P 318237-01-3P  
 318237-03-5P 318237-05-7P 318237-07-9P  
 318237-09-1P 318237-10-4P 318237-11-5P  
 318237-18-2P 318237-19-3P 318237-20-6P  
 318237-21-7P 318237-22-8P 318237-23-9P  
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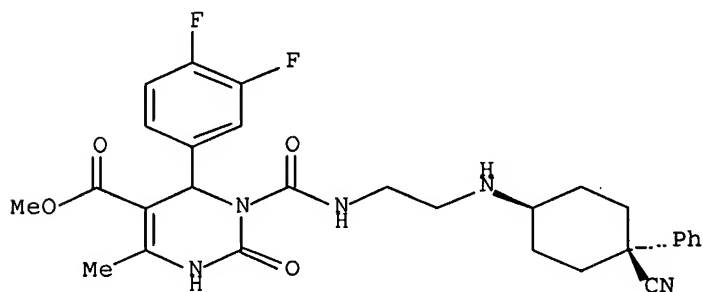
RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(preparation of dihydropyrimidines as selective antagonists for human  
 $\alpha 1A$  receptors)

RN 191353-49-8 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[(cis-4-cyano-4-  
 phenylcyclohexyl)amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-  
 1,2,3,6-tetrahydro-4-methyl-2-oxo-, methyl ester, monohydrochloride (9CI)  
 (CA INDEX NAME)

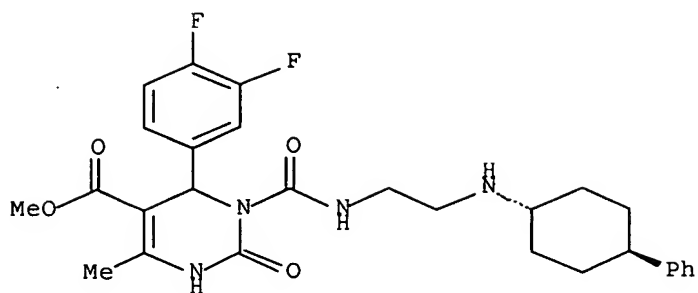
Relative stereochemistry.



● HCl

RN 191353-54-5 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[(cis-4-cyano-4-

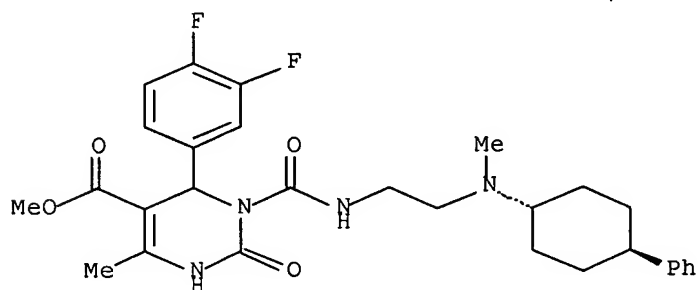


● HCl

RN 191353-58-9 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-methyl-1-[[[2-[methyl(trans-4-phenylcyclohexyl)amino]ethyl]amino]carbonyl]-2-oxo-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.

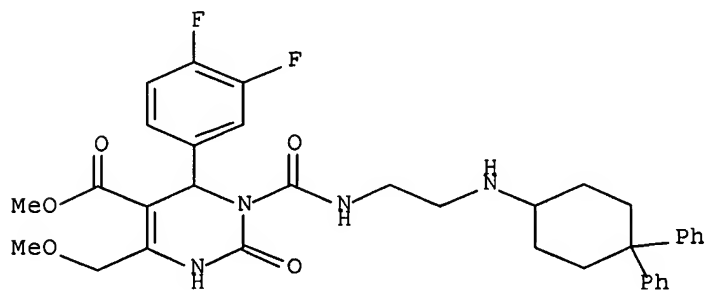


● HCl

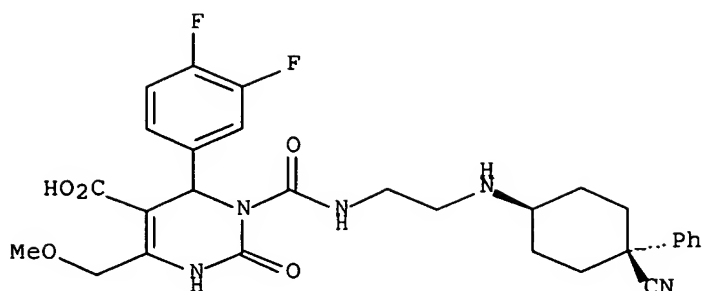
RN 191353-60-3 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1-[[[2-[(4,4-diphenylcyclohexyl)amino]ethyl]amino]carbonyl]-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, monohydrochloride, (+)- (9CI) (CA INDEX NAME)

Rotation (+).



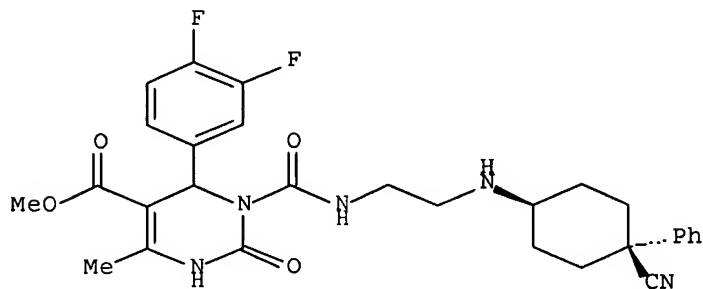
● HCl



RN 318236-90-7 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[(cis-4-cyano-4-phenylcyclohexyl)amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-, methyl ester (CA INDEX NAME)

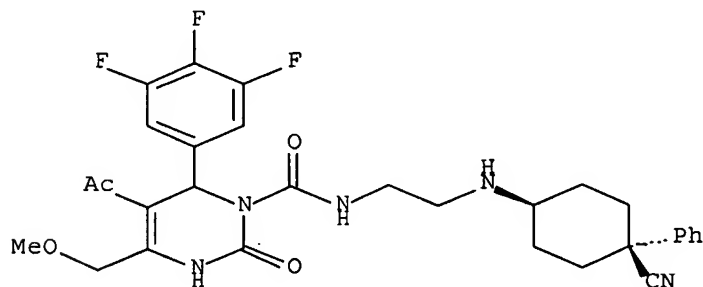
Relative stereochemistry.



RN 318236-91-8 HCAPLUS

CN 1(2H)-Pyrimidinecarboxamide, 5-acetyl-N-[2-[(cis-4-cyano-4-phenylcyclohexyl)amino]ethyl]-3,6-dihydro-4-(methoxymethyl)-2-oxo-6-(3,4,5-trifluorophenyl)- (CA INDEX NAME)

Relative stereochemistry.



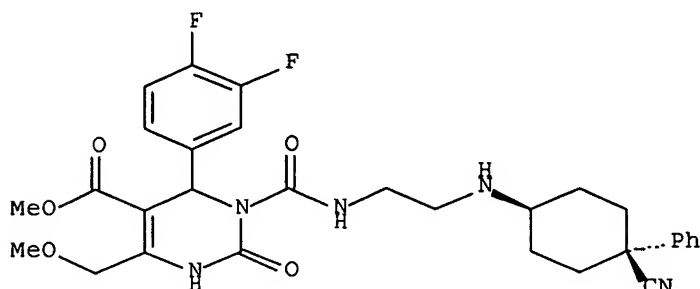
RN 318236-92-9 HCAPLUS

CN 1,5(6H)-Pyrimidinedicarboxamide, N1-[2-[(cis-4-cyano-4-phenylcyclohexyl)amino]ethyl]-6-(2,4-difluorophenyl)-4-ethyl-2,3-dihydro-2-oxo-, (+)- (9CI) (CA INDEX NAME)

RN 318236-95-2 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[(cis-4-cyano-4-phenylcyclohexyl)amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (-)- (CA INDEX NAME)

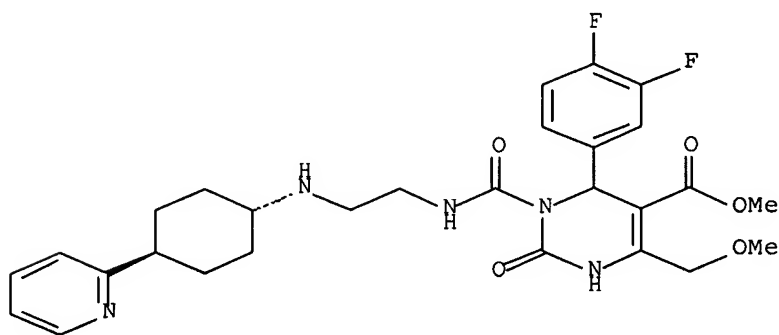
Rotation (-). Absolute stereochemistry unknown.



RN 318236-96-3 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-1-[[[2-[[trans-4-(2-pyridinyl)cyclohexyl]amino]ethyl]amino]carbonyl]-, methyl ester, (+)- (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

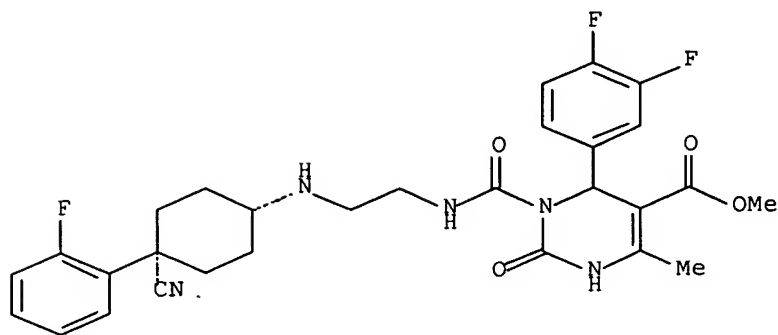


RN 318236-97-4 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-1-[[[2-[(cis-4-phenylcyclohexyl)amino]ethyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

Relative stereochemistry.

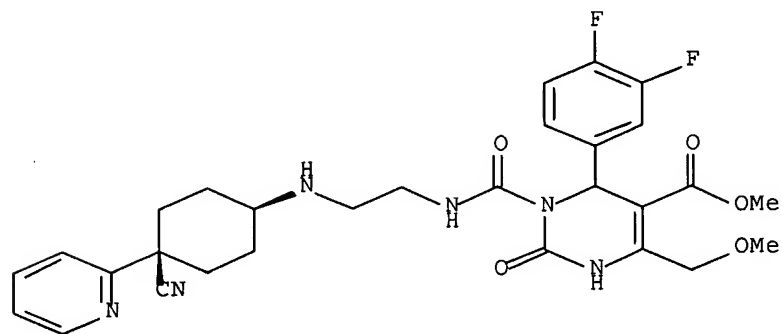
Rotation (+). Absolute stereochemistry unknown.



RN 318237-01-3 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[cis-4-cyano-4-(2-pyridinyl)cyclohexyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (+)- (CA INDEX NAME)

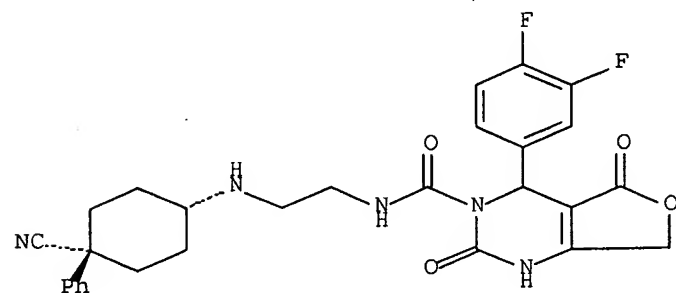
Rotation (+). Absolute stereochemistry unknown.

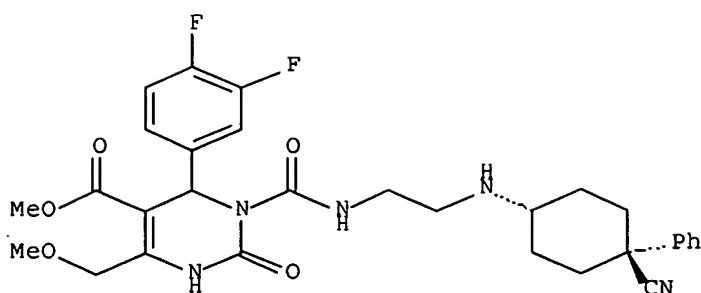


RN 318237-03-5 HCAPLUS

CN Furo[3,4-d]pyrimidine-3(4H)-carboxamide, N-[2-[(cis-4-cyano-4-phenylcyclohexyl)amino]ethyl]-4-(3,4-difluorophenyl)-1,2,5,7-tetrahydro-2,5-dioxo-, (+)- (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

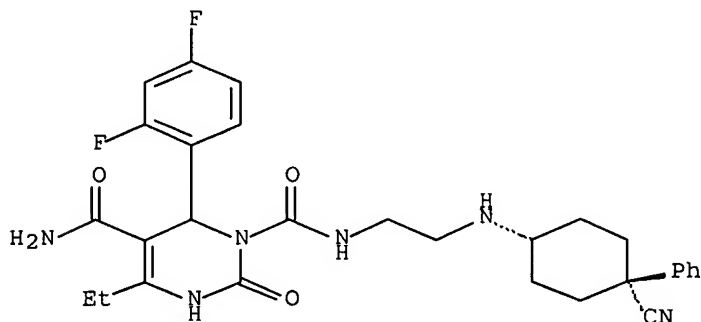




RN 318237-10-4 HCAPLUS

CN 1,5(6H)-Pyrimidinedicarboxamide, N1-[2-[(cis-4-cyano-4-phenylcyclohexyl)amino]ethyl]-6-(2,4-difluorophenyl)-4-ethyl-2,3-dihydro-2-oxo-, (9CI) (CA INDEX NAME)

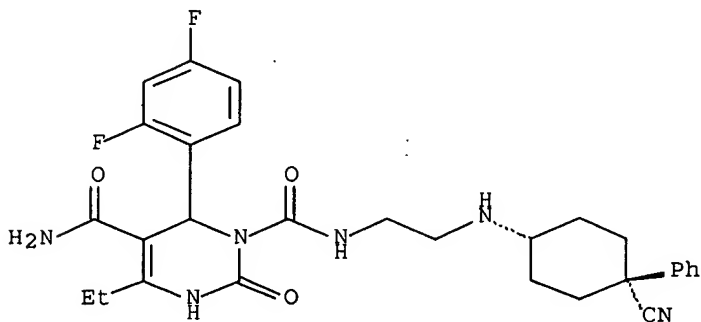
Relative stereochemistry.



RN 318237-11-5 HCAPLUS

CN 1,5(6H)-Pyrimidinedicarboxamide, N1-[2-[(cis-4-cyano-4-phenylcyclohexyl)amino]ethyl]-6-(2,4-difluorophenyl)-4-ethyl-2,3-dihydro-2-oxo-, (-) (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.



RN 318237-18-2 HCAPLUS

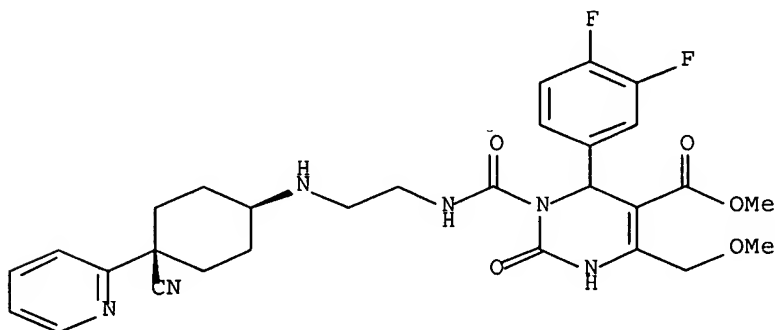
CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[(cis-4-cyano-4-(2-fluorophenyl)cyclohexyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-



RN 318237-21-7 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[cis-4-cyano-4-(2-pyridinyl)cyclohexyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (-)- (CA INDEX NAME)

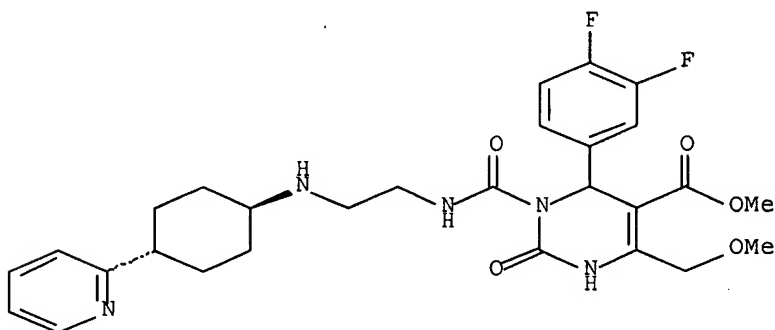
Rotation (-). Absolute stereochemistry unknown.



RN 318237-22-8 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-1-[[[2-[[trans-4-(2-pyridinyl)cyclohexyl]amino]ethyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

Relative stereochemistry.

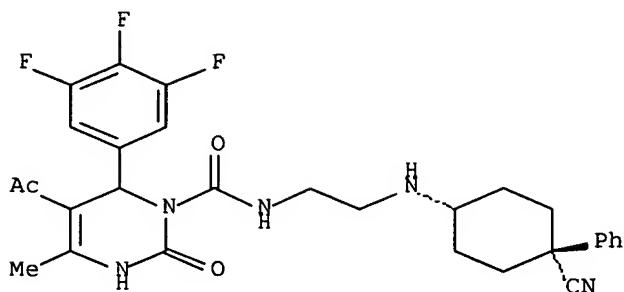


RN 318237-23-9 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-1-[[[2-[[trans-4-(2-pyridinyl)cyclohexyl]amino]ethyl]amino]carbonyl]-, methyl ester, (-)- (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.

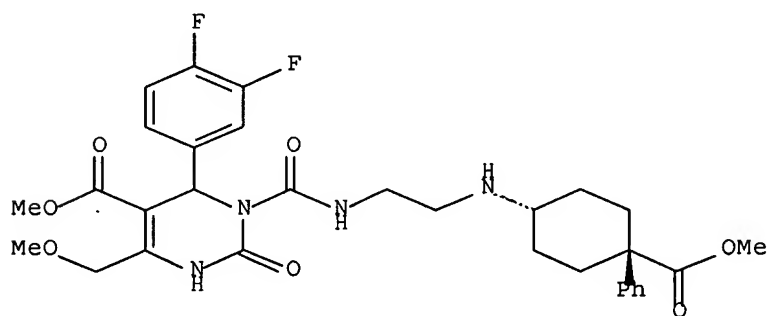
Rotation (-). Absolute stereochemistry unknown.



RN 318237-27-3 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-1-[[[2-[[cis-4-(methoxycarbonyl)-4-phenylcyclohexyl]amino]ethyl]amino]carbonyl]-4-(methoxymethyl)-2-oxo-, methyl ester (CA INDEX NAME)

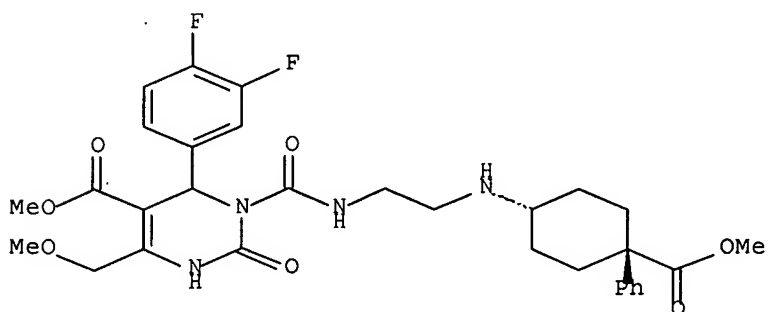
Relative stereochemistry.



RN 318237-28-4 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-1-[[[2-[[cis-4-(methoxycarbonyl)-4-phenylcyclohexyl]amino]ethyl]amino]carbonyl]-4-(methoxymethyl)-2-oxo-, methyl ester, (-)- (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.

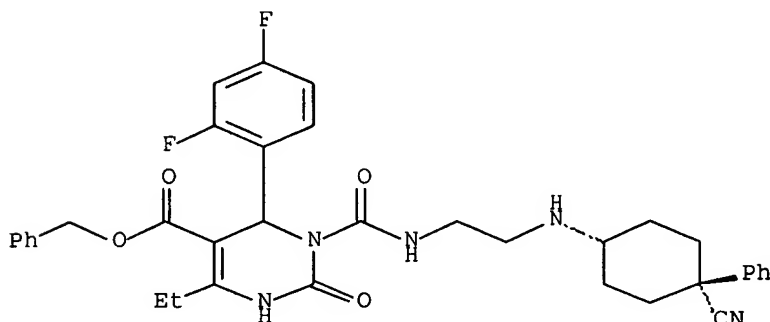


RN 338465-41-1 HCAPLUS

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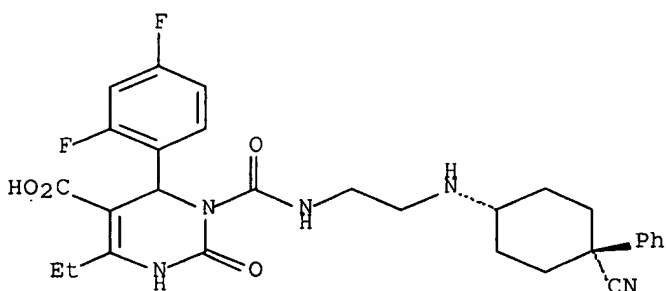
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 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of dihydropyrimidines as selective antagonists for human  
 $\alpha 1A$  receptors)  
 RN 318237-12-6 HCAPLUS  
 CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[(cis-4-cyano-4-  
 phenylcyclohexyl)amino]ethyl]amino]carbonyl]-6-(2,4-difluorophenyl)-4-  
 ethyl-1,2,3,6-tetrahydro-2-oxo-, phenylmethyl ester, (+)- (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



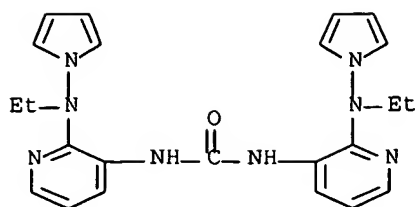
RN 318237-13-7 HCAPLUS  
 CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[(cis-4-cyano-4-  
 phenylcyclohexyl)amino]ethyl]amino]carbonyl]-6-(2,4-difluorophenyl)-4-  
 ethyl-1,2,3,6-tetrahydro-2-oxo-, (+)- (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



RN 338465-45-5 HCAPLUS  
 CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[(cis-4-cyano-4-  
 phenylcyclohexyl)amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-  
 1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, phenylmethyl ester, (+)- (CA  
 INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L167 ANSWER 8 OF 21 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:12266 HCAPLUS Full-text

DOCUMENT NUMBER: 134:86149

TITLE: Preparation of diphenyl ureas as VLA-4 inhibitors

INVENTOR(S): Baldwin, John J.; McDonald, Edward; Moriarty, Kevin Joseph; Sarko, Christopher Ronald; Machinaga, Nobuo; Nakayama, Atsushi; Chiba, Jun; Iimura, Shin; Yoneda, Yoshiyuki

PATENT ASSIGNEE(S): Daiichi Pharmaceutical Co., Ltd., Japan; Pharmacopeia, Inc.

SOURCE: PCT Int. Appl., 511 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001000206	A1	20010104	WO 2000-US18079	20000630 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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EP 1189612	A1	20020327	EP 2000-945035	20000630 <--
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JP 2003503350	T	20030128	JP 2001-505915	20000630 <--
AU 781438	B2	20050526	AU 2000-59031	20000630 <--
RU 2264386	C2	20051120	RU 2001-135856	20000630 <--
ZA 2001009203	A	20030207	ZA 2001-9203	20011107 <--
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US 7179819	B2	20070220		
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PRIORITY APPLN. INFO.:			US 1999-141601P	P 19990630 <--

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RL: BAC (Biological activity or effector, except adverse); BSU  
(Biological study, unclassified); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(preparation of di-Ph ureas as VLA-4 inhibitors)

IT	317354-42-0P	317354-43-1P	317354-44-2P	317354-45-3P	317354-46-4P
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RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(preparation of di-Ph ureas as VLA-4 inhibitors)

IT 99-42-3P, Methyl 4-hydroxy-3-nitrobenzoate 99-76-3P, Methyl  
 4-hydroxybenzoate 536-25-4P, Methyl 3-amino-4-hydroxybenzoate  
 614-78-8P 2495-37-6P 4560-41-2P, 2-Benzyloxynitrobenzene 5368-81-0P,  
 Methyl 3-methoxybenzoate 5985-24-0P, Dimethyl 4-hydroxyisophthalate  
 13143-00-5P 20012-63-9P, 2-Benzyloxyaniline 20986-40-7P 21784-73-6P,  
 4-Iodo-2-nitrophenol 23173-76-4P 26690-80-2P, 2-(N-tert-  
 Butoxycarbonylamino)ethanol 33165-09-2P, Ethyl 4-(2-  
 hydroxyethyl)piperazinyl-1-acetate 35387-92-9P, Methyl  
 4-iodo-3-methoxybenzoate 37669-64-0P 39741-46-3P 40004-08-8P, Ethyl  
 1-piperazinylacetate 41608-64-4P, Methyl 4-amino-3-methoxybenzoate  
 42923-79-5P 52274-10-9P 52928-01-5P 53088-68-9P 53542-91-9P  
 56850-93-2P, Methyl 4-(2-aminoethoxy)benzoate 56850-94-3P 57486-69-8P  
 57600-60-9P 59936-29-7P, N-tert-Butoxycarbonylproline methyl ester  
 63307-44-8P 66095-76-9P 66171-50-4P, Methyl 2-hydroxy-5-  
 pyridinecarboxylate 69610-40-8P 76254-70-1P 76587-66-1P  
 79069-13-9P, (S)-2-(N-tert-Butoxycarbonylamino)-1-propanol 80306-60-1P  
 80518-57-6P 84695-07-8P 84695-12-5P 93967-75-0P 97522-06-0P  
 101349-30-8P 102195-80-2P 106391-86-0P 111265-96-4P 113400-46-7P  
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 126550-68-3P 126550-70-7P 126550-71-8P 126550-73-0P 136235-11-5P  
 138528-06-0P 147266-79-3P 148626-26-0P 149814-40-4P 150529-73-0P,  
 Methyl 3-bromophenylacetate 160033-52-3P 170586-32-0P 171663-13-1P  
 173435-87-5P 177760-48-4P 181517-99-7P 181518-40-1P 183059-24-7P  
 185200-33-3P, Methyl 3-bromo-4-nitrophenylacetate 185951-13-7P  
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 Benzyl (S)-4-(2-amino-1-propoxy)benzoate 316129-59-6P 316134-67-5P,  
 Ethyl 4-(2-bromoethyl)piperazinyl-1-acetate 316135-69-0P 316137-55-0P  
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317819-94-6P 317819-95-7P 317819-96-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of di-Ph ureas as VLA-4 inhibitors)

IT 317354-29-3P 317354-33-9P 317354-48-6P

317354-49-7P 317362-82-6P 317362-85-9P

317362-86-0P 317362-92-8P

RL: BAC (Biological activity or effector, except adverse); BSU

(Biological study, unclassified); SPN (Synthetic preparation); THU

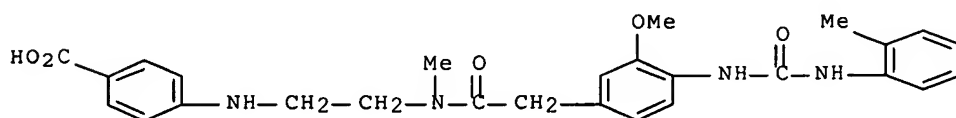
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(Uses)

(preparation of di-Ph ureas as VLA-4 inhibitors)

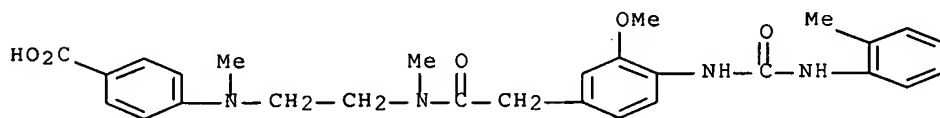
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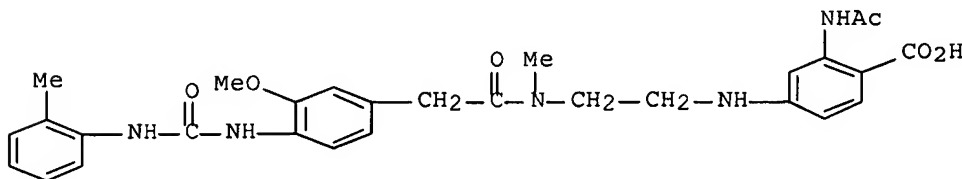
RN 317354-33-9 HCAPLUS

CN Benzoic acid, 4-[[2-[[[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]acetyl]methylamino]ethyl]amino]- (9CI) (CA INDEX NAME)



RN 317354-48-6 HCAPLUS

CN Benzoic acid, 2-(acetylamino)-4-[[2-[[[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]acetyl]methylamino]ethyl]amino]- (9CI) (CA INDEX NAME)



RN 317354-49-7 HCAPLUS

CN Benzoic acid, 2-(acetylamino)-4-[[2-[[[4-[[[(2-bromophenyl)amino]carbonyl]amino]-3-methoxyphenyl]acetyl]methylamino]ethyl]amino]- (9CI) (CA INDEX NAME)

IT 317355-02-5P 317359-43-6P 317359-75-4P

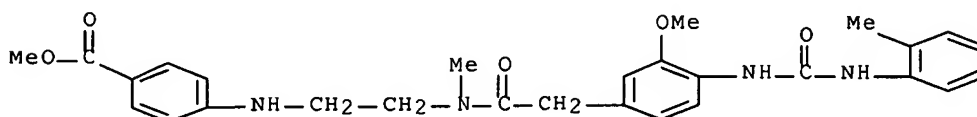
317359-76-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of di-Ph ureas as VLA-4 inhibitors)

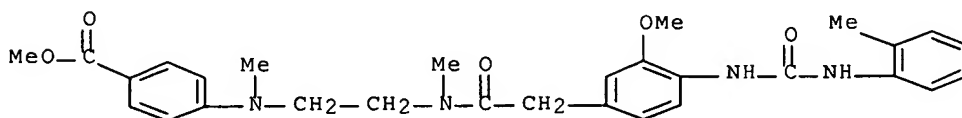
RN 317355-02-5 HCAPLUS

CN Benzoic acid, 4-[[2-[[[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]acetyl]methylamino]ethyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



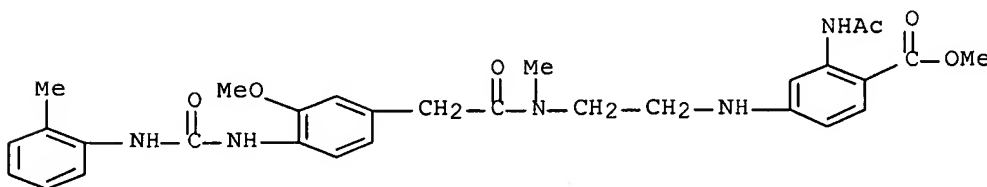
RN 317359-43-6 HCAPLUS

CN Benzoic acid, 4-[[2-[[[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]acetyl]methylamino]ethyl]methylamino]-, methyl ester (9CI) (CA INDEX NAME)



RN 317359-75-4 HCAPLUS

CN Benzoic acid, 2-(acetylamino)-4-[[2-[[[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]acetyl]methylamino]ethyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



RN 317359-76-5 HCAPLUS

CN Benzoic acid, 2-(acetylamino)-4-[[2-[[[4-[[[(2-bromophenyl)amino]carbonyl]amino]-3-methoxyphenyl]acetyl]methylamino]ethyl]amino]-, methyl ester (9CI) (CA INDEX NAME)



ES 2261844	T3	20061116	ES 2003-23514	19990805 <--
PT 1380582	T	20060831	PT 2003-23514	19990808 <--
US 6423723	B1	20020723	US 2000-723495	20001128 <--
US 2002147345	A1	20021010	US 2002-156431	20020528 <--
US 6653338	B2	20031125	.	
AU 2004202858	A1	20040722	AU 2004-202858	20040625 <--
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			EP 1999-939686	A3 19990805 <--
			US 1999-369222	A3 19990805 <--
			WO 1999-US17755	W 19990805 <--
			US 2000-723495	A3 20001128 <--

OTHER SOURCE(S): MARPAT 132:151680

AB R5ZYR4XR3WNR1R2 [R1, R3, R4, R5 = H, (substituted) alkyl, alkenyl, alkynyl, alkoxy, alkoxy carbonyl, thioalkyl, acyl, acyloxy, aryl, cycloalkyl, heterocyclyl; R2 = H, (substituted) cycloalkyl, heterocyclyl, aryl, heteroaryl; NR1R2 = (substituted) heterocyclyl, heteroaryl; W = CO, NHCO, NHCOCH2, C:NH, CS, SO2, (substituted) CH2; X, Y = CH, N; Z = CO, NH, C:N, SO2, CONH], were prepared Thus, 1-[(2-oxo-6-pentyl-2H-pyran)-3-carbonyl]pyrrolidine-2-carboxylic acid 3-(9-ethylcarbazolyl)amide (prepared from BOC-Pro-OH, 3-amino-9-ethylcarbazole, and 2-oxo-6-pentyl-2H-pyran-3-carboxylic acid) stimulated estradiol production in the rat granulosa cell assay with EC50 = 1.4  $\mu$ M.

IC ICM C07D405-00

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1, 2, 34

IT 258277-64-4P 258277-65-5P 258277-66-6P 258277-67-7P 258277-68-8P  
 258277-69-9P 258277-70-2P 258277-71-3P 258277-72-4P 258277-73-5P  
 258277-74-6P 258277-75-7P 258277-76-8P 258277-77-9P 258277-78-0P  
 258277-79-1P 258277-80-4P 258277-81-5P 258277-82-6P 258277-83-7P  
 258277-84-8P 258277-85-9P 258277-86-0P 258277-87-1P 258277-88-2P  
 258277-89-3P 258277-90-6P 258277-91-7P 258277-93-9P 258277-95-1P  
 258277-96-2P 258277-97-3P 258277-98-4P 258277-99-5P 258278-00-1P  
 258278-01-2P 258278-02-3P 258278-03-4P 258278-04-5P 258278-06-7P  
 258278-07-8P 258278-08-9P 258278-09-0P 258278-10-3P 258278-11-4P  
 258278-12-5P 258278-13-6P 258278-14-7P 258278-17-0P  
 258278-18-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of carbazoles, isoquinolines, indoles, and related compds. as FSH mimetics for the treatment of infertility)

IT 258278-13-6P 258278-14-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of carbazoles, isoquinolines, indoles, and related compds. as FSH mimetics for the treatment of infertility)

RN 258278-13-6 HCAPLUS

CN 2H-Pyran-3-carboxamide, N-[2-[(9-ethyl-9H-carbazol-3-yl)amino]-3-pyridinyl]-2-oxo-6-pentyl- (CA INDEX NAME)

frontal cortex membranes containing serotonin 5-HT<sub>1A</sub> receptors in vitro. The compds. displayed weak to high affinities for dopamine D<sub>2</sub> receptors, with K<sub>i</sub>-values ranging from 550 nM for the 5-carboxamido analog to 4.9 nM for the 5-hydroxy analog. The relative affinities of the 5-methoxy, 5-hydroxy, and 5-unsubstituted analogs suggested that these compds. may bind to the same site and in a similar way as the 5-oxygenated DPATs, with the 5-methoxy substituent of I functioning as a hydrogen bond acceptor. The serotonin 5-HT<sub>1A</sub> receptor tolerated more structural diversity at the C5-position of I, as revealed by the higher K<sub>i</sub>-values which ranged from 60 nM for the 5-carboxamido analog to 1.0 nM for the 5-unsubstituted analog. Partial least-squares (PLS) anal. of a set of 24 mol. descriptors, generated for each analog, revealed no significant correlation between the dopamine D<sub>2</sub> receptor affinities of the compds. and their mol. properties, supporting the view that they may have different binding modes at this receptor subtype. A PLS model with moderate predictability (Q<sub>2</sub> = 0.49) could be derived for the serotonin 5-HT<sub>1A</sub> receptor affinities of the compds. studied. According to the model, a relatively lipophilic, nonpolar C5-substituent should be optimal for a high affinity at this receptor subtype.

- CC 1-3 (Pharmacology)  
Section cross-reference(s): 25
- IT 257294-06-7P 257294-13-6P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation and interactions with dopamine D<sub>2</sub> and serotonin 5-HT<sub>1A</sub> receptors of benzamide aminotetralin derivs.)
- IT 257294-04-5  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)  
(preparation and interactions with dopamine D<sub>2</sub> and serotonin 5-HT<sub>1A</sub> receptors of benzamide aminotetralin derivs.)
- IT 257294-07-8P 257294-08-9P 257294-09-0P  
257294-10-3P 257294-11-4P 257294-12-5P  
257294-14-7P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation and interactions with dopamine D<sub>2</sub> and serotonin 5-HT<sub>1A</sub> receptors of benzamide aminotetralin derivs.)
- IT 220772-95-2 257294-05-6  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(preparation and interactions with dopamine D<sub>2</sub> and serotonin 5-HT<sub>1A</sub> receptors of benzamide aminotetralin derivs.)
- IT 257294-06-7P 257294-13-6P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation and interactions with dopamine D<sub>2</sub> and serotonin 5-HT<sub>1A</sub> receptors of benzamide aminotetralin derivs.)
- RN 257294-06-7 HCAPLUS
- CN Methanesulfonic acid, trifluoro-, 6-[[2-(benzoylamino)ethyl]propylamino]-5,6,7,8-tetrahydro-1-naphthalenyl ester (9CI) (CA INDEX NAME)

(Biological study, unclassified); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(preparation and interactions with dopamine D2 and serotonin 5-HT1A  
receptors of benzamide aminotetralin derivs.)

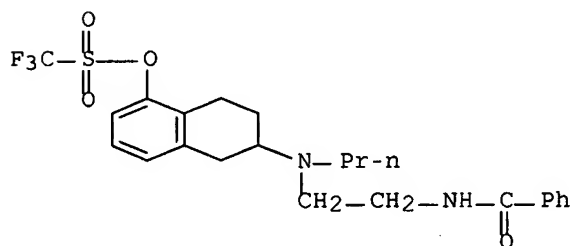
RN 257294-07-8 HCAPLUS

CN Methanesulfonic acid, trifluoro-, 6-[[2-(benzoylamino)ethyl]propylamino]-  
5,6,7,8-tetrahydro-1-naphthalenyl ester, ethanedioate (1:1) (9CI) (CA  
INDEX NAME)

CM 1

CRN 257294-06-7

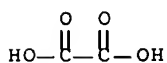
CMF C23 H27 F3 N2 O4 S



CM 2

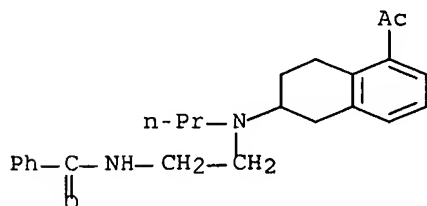
CRN 144-62-7

CMF C2 H2 O4



RN 257294-08-9 HCAPLUS

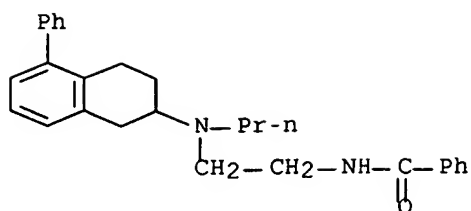
CN Benzamide, N-[2-[(5-acetyl-1,2,3,4-tetrahydro-2-  
naphthalenyl)propylamino]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 257294-09-0 HCAPLUS

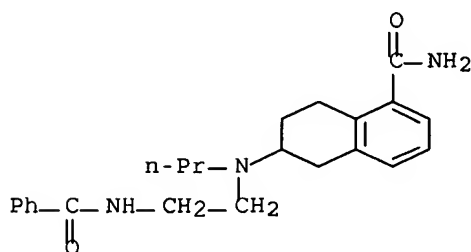
CN Benzamide, N-[2-[(5-cyano-1,2,3,4-tetrahydro-2-



● HCl

RN 257294-14-7 HCAPLUS

CN 1-Naphthalenecarboxamide, 6-[[2-(benzoylamino)ethyl]propylamino]-5,6,7,8-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

IT 220772-95-2 257294-05-6

RL: BAC (Biological activity or effector, except adverse); BSU

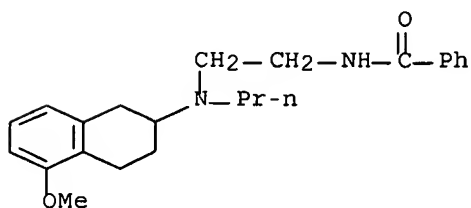
(Biological study, unclassified); THU (Therapeutic use); BIOL

(Biological study); USES (Uses)

(preparation and interactions with dopamine D2 and serotonin 5-HT1A receptors of benzamide aminotetralin derivs.)

RN 220772-95-2 HCAPLUS

CN Benzamide, N-[2-[propyl(1,2,3,4-tetrahydro-5-methoxy-2-naphthalenyl)amino]ethyl]- (CA INDEX NAME)

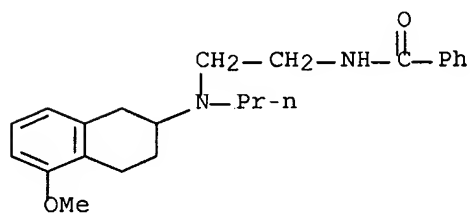


RN 257294-05-6 HCAPLUS

CN Benzamide, N-[2-[propyl(1,2,3,4-tetrahydro-2-naphthalenyl)amino]ethyl]- (CA INDEX NAME)

production in GH4ZD10 cells expressing serotonin 5-HT1A receptors. Both enantiomers of I (R = H) behaved as full serotonin 5-HT1A receptor agonists in this assay, while both enantiomers of I (R = MeO) behaved as weak partial agonists. The potential antipsychotic properties of (S)- and (R)-I (R = H) were evaluated by establishing their ability to inhibit d-amphetamine-induced locomotor activity in rats, while their propensity to induce extrapyramidal side-effects (EPS) in man was evaluated by determining their ability to induce catalepsy in rats. Whereas (R)-I (R = H) was capable of blocking d-amphetamine-induced locomotor activity, indicative of dopamine D2 receptor antagonism, (S)-I (R = H) even enhanced the effect of d-amphetamine, suggesting that this compound has dopamine D2 receptor-stimulating properties. Since both enantiomers of I (R = H) also were devoid of cataleptogenic activity, they are interesting candidates for further exploring the dopamine D2/serotonin 5-HT1A hypothesis of atypical antipsychotic drug action.

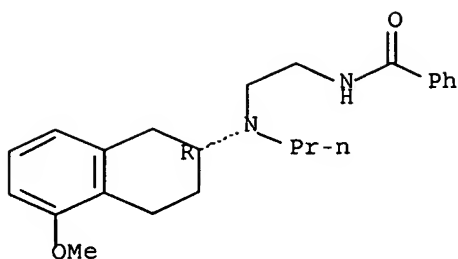
- CC 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
Section cross-reference(s): 1
- IT 220772-98-5 244239-82-5  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
(preparation of propylbenzoylaminotetralins and their enantiomers as potential antipsychotic agents and their binding to adrenergic, dopamine, and serotonin receptors)
- IT 590-17-0P, Bromoacetonitrile 244239-70-1P 244239-72-3P  
244239-75-6P 244239-76-7P 244239-78-9P  
244239-80-3P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of propylbenzoylaminotetralins and their enantiomers as potential antipsychotic agents and their binding to adrenergic, dopamine, and serotonin receptors)
- IT 220772-98-5 244239-82-5  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
(preparation of propylbenzoylaminotetralins and their enantiomers as potential antipsychotic agents and their binding to adrenergic, dopamine, and serotonin receptors)
- RN 220772-98-5 HCAPLUS
- CN Benzamide, N-[2-[propyl(1,2,3,4-tetrahydro-5-methoxy-2-naphthalenyl)amino]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

- RN 244239-82-5 HCAPLUS
- CN Benzamide, 2,6-dimethoxy-N-[2-[propyl(1,2,3,4-tetrahydro-5-methoxy-2-naphthalenyl)amino]ethyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1



● HCl

RN 244239-78-9 HCAPLUS

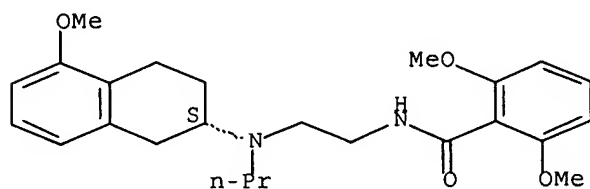
CN Benzamide, 2,6-dimethoxy-N-[2-[propyl[(2S)-1,2,3,4-tetrahydro-5-methoxy-2-naphthalenyl]amino]ethyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 244239-77-8

CMF C25 H34 N2 O4

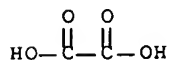
Absolute stereochemistry. Rotation (-).



CM 2

CRN 144-62-7

CMF C2 H2 O4



RN 244239-80-3 HCAPLUS

CN Benzamide, 2,6-dimethoxy-N-[2-[propyl[(2R)-1,2,3,4-tetrahydro-5-methoxy-2-naphthalenyl]amino]ethyl]-, ethanedioate (1:1) (CA INDEX NAME)

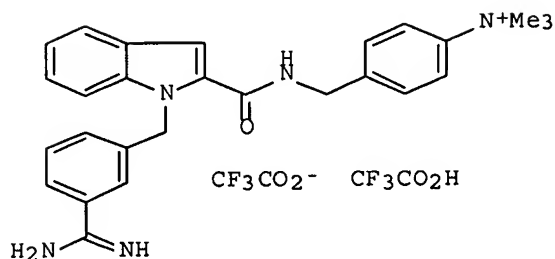
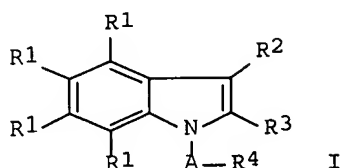
CM 1

CRN 244239-79-0

CMF C25 H34 N2 O4

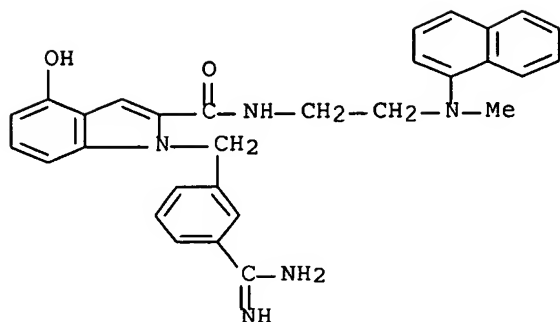
Absolute stereochemistry. Rotation (+).

TR 200001954	T2	20001221	TR 2000-1954	19981210 <--
HU 2001000723	A2	20010828	HU 2001-723	19981210 <--
HU 2001000723	A3	20021228		
JP 2001527066	T	20011225	JP 2000-526484	19981210 <--
NZ 505370	A	20020628	NZ 1998-505370	19981210 <--
RU 2225397	C2	20040310	RU 2000-119774	19981210 <--
AT 293599	T	20050515	AT 1998-965244	19981210 <--
ES 2241194	T3	20051016	ES 1998-965244	19981210 <--
PL 195682	B1	20071031	PL 1998-341400	19981210 <--
ZA 9811759	A	19990728	ZA 1998-11759	19981222 <--
TW 241294	B	20051011	TW 1998-87121374	19990223 <--
MX 2000PA05706	A	20010219	MX 2000-PA5706	20000609 <--
NO 2000003057	A	20000818	NO 2000-3057	20000614 <--
NO 316912	B1	20040621		
IN 2000CN00135	A	20050304	IN 2000-CN135	20000621 <--
US 6337344	B1	20020108	US 2000-582344	20000814 <--
HK 1033795	A1	20060113	HK 2001-104324	20010621 <--
PRIORITY APPLN. INFO.:			EP 1997-122901	A 19971224 <--
			WO 1998-EP8030	W 19981210 <--
OTHER SOURCE(S):	MARPAT	131:87814		
GI				



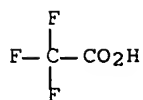
AB The invention relates to the inhibition of blood clotting proteins, and more particularly, to indole derivs. or their physiol. acceptable salts which effect this, having formula I [R1 groups = H, halo, alkyl, CF3, (un)substituted Ph or phenylalkoxy, etc., with  $\geq 2$  of R1 being H;  $\geq 1$  of R2 and R3 = (CH<sub>2</sub>)<sub>0-2</sub>CO<sub>2</sub>H or derivs., other = H, F, Cl, Br, or alkyl; or R2R3 = CH<sub>2</sub>CH<sub>2</sub>N(COPh)CH<sub>2</sub> or analogs; A = bond, alk(en/yn)ylene, CO, SO, SO<sub>2</sub>, etc.; R4 = (un)substituted Ph, pyridyl, or other heterocyclyl]. I are inhibitors of the blood clotting enzyme factor Xa. The invention also relates to processes for the preparation of I, to methods of inhibiting factor Xa activity and blood clotting, to use of I in the treatment and prophylaxis of associated (e.g., thromboembolic) diseases, and to the use of I in the preparation of related medicaments. The invention further relates to compns. containing I, in particular pharmaceutical compns. containing a compound I and pharmaceutically acceptable carriers and/or auxiliary substances. Over 160

CRN 229953-07-5  
CMF C30 H29 N5 O2



CM 2

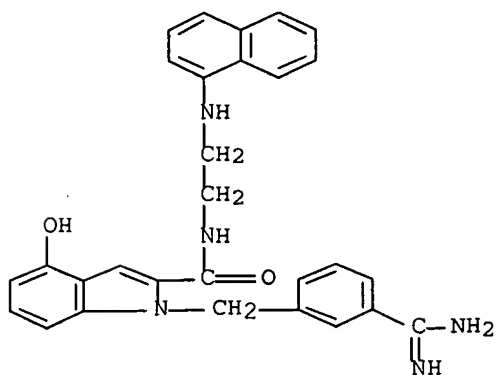
CRN 76-05-1  
CMF C2 H F3 O2



RN 229953-10-0 HCAPLUS  
CN 1H-Indole-2-carboxamide, 1-[[3-(aminoiminomethyl)phenyl]methyl]-4-hydroxy-  
N-[2-(1-naphthalenylamino)ethyl]-, mono(trifluoroacetate) (salt) (9CI)  
(CA INDEX NAME)

CM 1

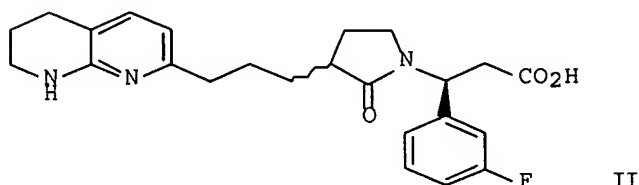
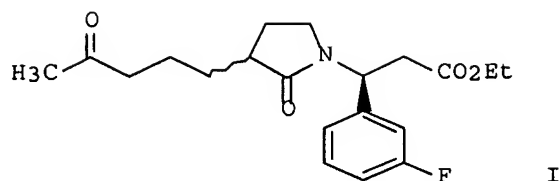
CRN 229953-09-7  
CMF C29 H27 N5 O2





US 1998-79944P	P	19980330 <--
US 1998-80397P	P	19980402 <--
GB 1998-10882	A	19980520 <--
GB 1998-10892	A	19980520 <--
GB 1998-12686	A	19980612 <--
US 1998-92624P	P	19980713 <--
US 1998-99948P	P	19980911 <--
GB 1998-22331	A	19981013 <--
GB 1998-22701	A	19981016 <--
JP 2000-539023	A3	19981214 <--
WO 1998-US26539	W	19981214 <--
US 1998-212123	A3	19981215 <--

OTHER SOURCE(S):            MARPAT 131:58814  
GI



AB The invention relates to compds. and derivs. thereof, their synthesis, and their use as vitronectin receptor antagonists. Representative compds. include those of formula W-X-Y-Z-CR5R6-CR7R8-CO2R9 [W = (un)substituted formamidino or guanidino, or various (poly)cyclic groups; X = (un)substituted linear alkylene, or a carbo- or heterocyclic group; Y = (un)substituted linear alkylene or hetero derivs. thereof; Z = (un)substituted carbo- or heterocyclic group; R5-R8 = H or a wide variety of simple or complex substituents; R9 = H, alkyl, aryl, aralkyl, etc.]. More particularly, the compds. are antagonists of the vitronectin receptors  $\alpha\beta3$ ,  $\alpha\beta5$ , and/or  $\alpha\beta6$ , and are useful for inhibiting bone resorption, treating and preventing osteoporosis, and inhibiting vascular restenosis, diabetic retinopathy, macular degeneration, angiogenesis, atherosclerosis, inflammation, viral disease, and tumor growth. The compds. typically display sub- micromolar affinity for integrin receptors, particularly  $\alpha\beta3$ ,  $\alpha\beta5$ , and/or  $\alpha\beta6$  receptors (no data). For instance, the intermediate I (preparation given) underwent a sequence of: (1) cyclocondensation with 2-amino-3-formylpyridine to form a 1,8-naphthyridine nucleus, (2) hydrogenation of the latter to a tetrahydro derivative; and (3) alkaline hydrolysis of the ester, to give two diastereomeric products II, which were separated by chromatog.

IC ICM A61K031-435

ICS A61K031-40; C07D207-26; C07D413-06; C07D471-04; C07D401-06

CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

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WO 9857638          A1      19981223      WO 1998-US12567      19980617 <--
W:  AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, GW,
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    MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA,
    US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,
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CA 2294590          A1      19981223      CA 1998-2294590      19980617 <--
AU 9879726          A      19990104      AU 1998-79726      19980617 <--
EP 1023068          A1      20000802      EP 1998-930307      19980617 <--
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JP 2002511085       T      20020409      JP 1999-504715      19980617 <--
US 6376503          B1      20020423      US 1998-97947      19980617 <--
PRIORITY APPLN. INFO.:
                                US 1997-50959P      P 19970618 <--
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                                WO 1998-US12567      W 19980617 <--

OTHER SOURCE(S):          MARPAT 130:81519
GI

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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The title compds. [I;Q = II-IV, etc.; E, G, L, M = H, C1-8 alkyl, C3-8 cycloalkyl, etc.; J = H, C1-8 alkyl, C3-8 cycloalkyl, etc.; R1 = (un)substituted Ph, pyridyl, pyrazinyl, etc.; R2, R7 = H, C1-8 alkyl, C4-8 cycloalkyl, etc.; R3, R6, R9, R10 = H, C1-8 alkyl, C3-8 cycloalkyl, etc.; R4 = H, (CH2)0-4CN, (CH2)0-4CF3, etc.; R5, R8 = H, C1-8 alkyl, C3-8 cycloalkyl, etc.; m, n, q = 0-4; o = 2-5; r = 0-1], alpha 1a adrenergic receptor antagonists which are useful in the treatment of benign prostatic hyperplasia, were prepared. Thus, reaction of pyrimidinone V with N1-[1-(2-nitrophenyl)piperidin-4-yl]ethane-1,2-diamine in CH2Cl2 afforded the title compound (4S)-VI. Representative compds. I were found to have Ki of ≤ 50 nM against alpha 1a adrenergic receptor binding. The compds. I are selective in their ability to relax smooth muscle tissue enriched in the alpha 1a receptor subtype without at the same time inducing hypotension. One such tissue is found surrounding the urethral lining. Therefore, one utility of the instant compds. is to provide acute relief to males suffering from benign prostatic hyperplasia, by permitting less hindered urine flow. Another utility of the instant compds. I is provided by combination with a human 5-alpha reductase inhibitory compound, such that both acute and chronic relief from the effects of benign prostatic hyperplasia are achieved.

IC ICM A61K031-445  
ICS A61K031-505; C07D211-18; C07D239-34; C07D491-08; C07D487-04;  
C07D401-12; C07D411-12; C07D413-12

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1

IT 218609-83-7P 218610-00-5P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of [2-(piperidin-4-yl)aminoethylcarbamoyl] substituted 1,2,3,4-tetrahydropyrimidines and oxazolidines as alpha 1a adrenergic receptor antagonists)

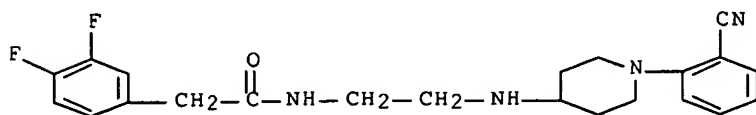
IT 218603-62-4P 218603-82-8P 218609-03-1P  
218609-04-2P 218609-05-3P 218609-06-4P

PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of [2-(piperidin-4-yl)aminoethylcarbamoyl] substituted  
1,2,3,4-tetrahydropyrimidines and oxazolidines as alpha 1a adrenergic  
receptor antagonists)

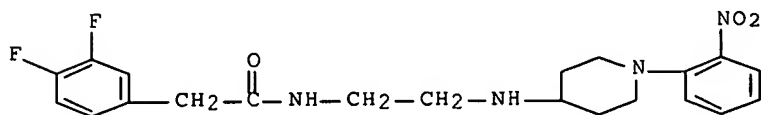
RN 218609-83-7 HCAPLUS

CN Benzeneacetamide, N-[2-[[1-(2-cyanophenyl)-4-piperidinyl]amino]ethyl]-3,4-  
difluoro- (CA INDEX NAME)



RN 218610-00-5 HCAPLUS

CN Benzeneacetamide, 3,4-difluoro-N-[2-[[1-(2-nitrophenyl)-4-piperidinyl]amino]ethyl]- (CA INDEX NAME)

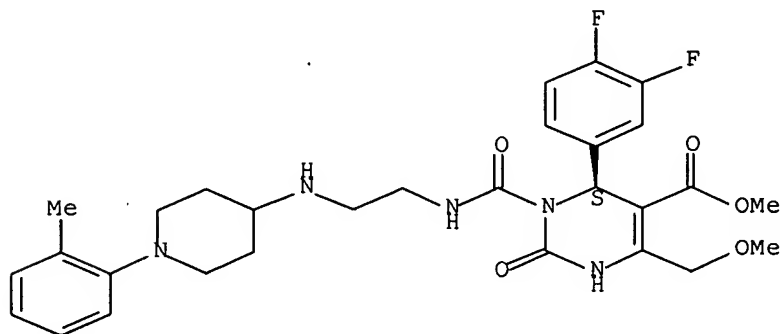


IT 218603-62-4P 218603-82-8P 218609-03-1P  
218609-04-2P 218609-05-3P 218609-06-4P  
218609-07-5P 218609-08-6P 218609-09-7P  
218609-10-0P 218609-12-2P 218609-13-3P  
218609-14-4P 218609-15-5P 218609-17-7P  
218609-18-8P 218609-19-9P 218609-20-2P  
218609-21-3P 218609-22-4P 218609-23-5P  
218609-25-7P 218609-26-8P 218609-27-9P  
218609-28-0P 218609-29-1P 218609-30-4P  
218609-31-5P 218609-32-6P 218609-33-7P  
218609-35-9P 218609-36-0P 218609-37-1P  
218609-39-3P 218609-40-6P 218609-41-7P  
218609-42-8P 218609-43-9P 218609-44-0P  
218609-45-1P 218609-46-2P 218609-47-3P  
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218609-62-2P 218609-63-3P 218609-64-4P  
218609-65-5P 218609-66-6P 218609-67-7P  
218609-69-9P 218609-70-2P 218609-71-3P  
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218609-78-0P 218609-79-1P 218609-80-4P  
218609-81-5P 218609-82-6P 218609-84-8P  
218609-85-9P 218609-86-0P 218609-87-1P  
218609-89-3P 218609-90-6P 218609-91-7P  
218609-92-8P 218609-93-9P 218609-95-1P  
218609-97-3P 218609-98-4P 218609-99-5P  
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218610-06-1P 218610-07-2P 218610-08-3P

RN 218609-03-1 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-1-[[[2-[[1-(2-methylphenyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-2-oxo-, methyl ester, monohydrochloride, (6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

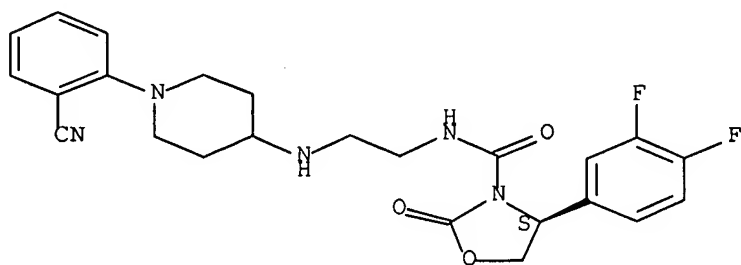


● HCl

RN 218609-04-2 HCAPLUS

CN 3-Oxazolidinecarboxamide, N-[2-[[1-(2-cyanophenyl)-4-piperidinyl]amino]ethyl]-4-(3,4-difluorophenyl)-2-oxo-, monohydrochloride, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

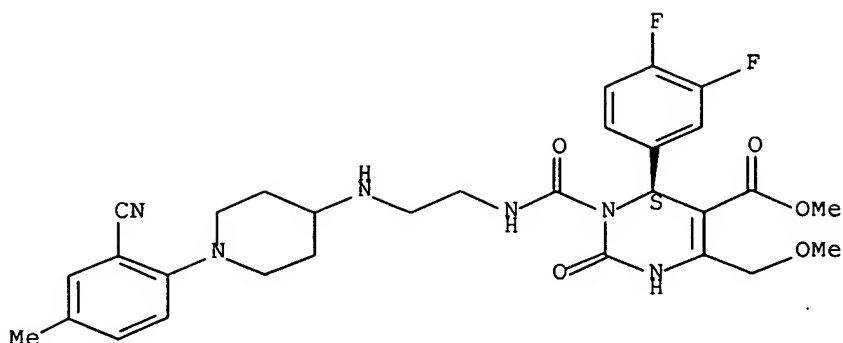


● HCl

RN 218609-05-3 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-1-[[[2-[[1-(2-methoxyphenyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-2-oxo-, methyl ester, dihydrochloride, (6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

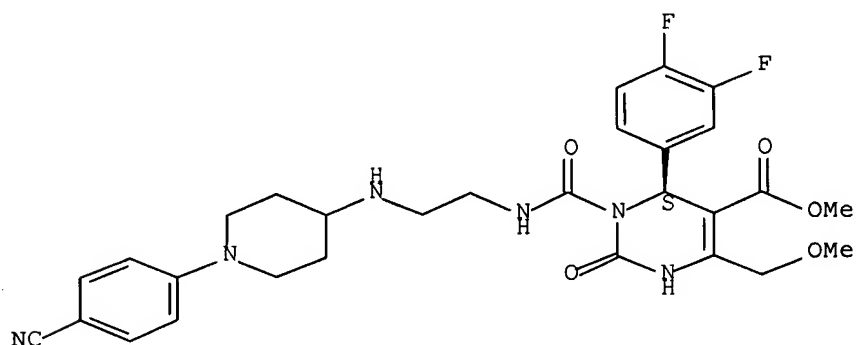


● HCl

RN 218609-08-6 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-(4-cyanophenyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, monohydrochloride, (6S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

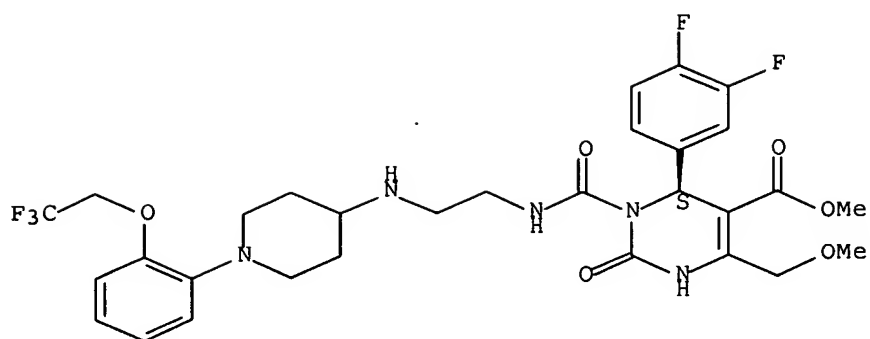


● HCl

RN 218609-09-7 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-(2-cyano-4-fluorophenyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, monohydrochloride, (6S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

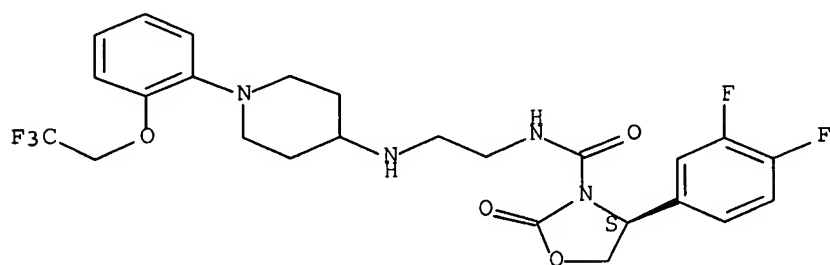


● HCl

RN 218609-13-3 HCAPLUS

CN 3-Oxazolidinecarboxamide, 4-(3,4-difluorophenyl)-2-oxo-N-[2-[[1-[2-(2,2,2-trifluoroethoxy)phenyl]-4-piperidinyl]amino]ethyl]-, monohydrochloride, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

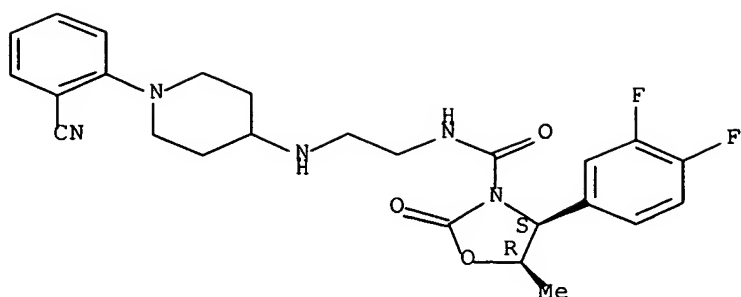


● HCl

RN 218609-14-4 HCAPLUS

CN 3-Oxazolidinecarboxamide, N-[2-[[1-(2-cyanophenyl)-3-pyrrolidinyl]amino]ethyl]-4-(3,4-difluorophenyl)-2-oxo-, monohydrochloride, (4S)- (9CI) (CA INDEX NAME)

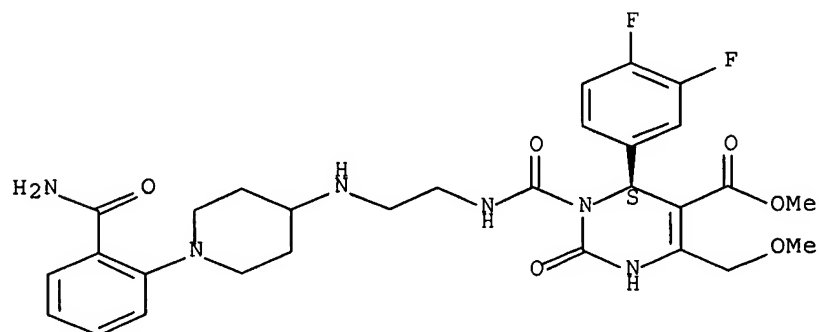
Absolute stereochemistry.



RN 218609-18-8 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-[2-(aminocarbonyl)phenyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

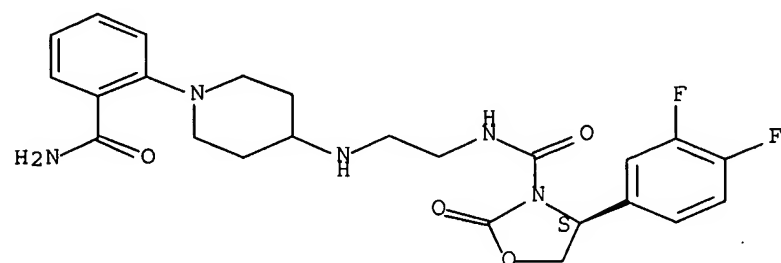
Absolute stereochemistry.



RN 218609-19-9 HCAPLUS

CN 3-Oxazolidinecarboxamide, N-[2-[[1-[2-(aminocarbonyl)phenyl]-4-piperidinyl]amino]ethyl]-4-(3,4-difluorophenyl)-2-oxo-, dihydrochloride, (4S)- (9CI) (CA INDEX NAME)

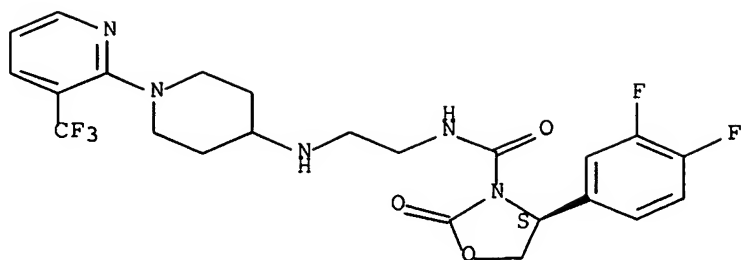
Absolute stereochemistry.



● 2 HCl

RN 218609-20-2 HCAPLUS

CN Benzoic acid, 2-[4-[[2-[[[(4S)-4-(3,4-difluorophenyl)-2-oxo-3-



RN 218609-23-5 HCAPLUS

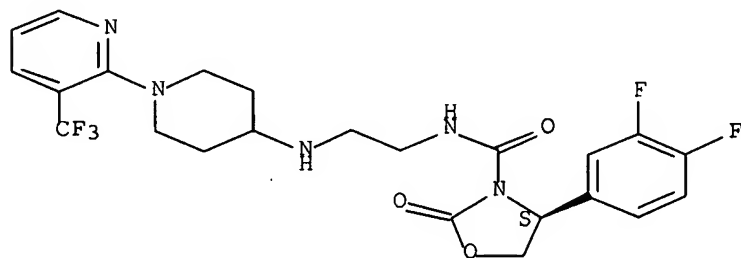
CN 3-Oxazolidinecarboxamide, 4-(3,4-difluorophenyl)-2-oxo-N-[2-[[1-[3-(trifluoromethyl)-2-pyridinyl]-4-piperidinyl]amino]ethyl]-, (4S)-, trifluoroacetate (2:3) (9CI) (CA INDEX NAME)

CM 1

CRN 218609-22-4

CMF C23 H24 F5 N5 O3

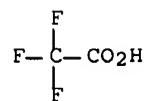
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 218609-25-7 HCAPLUS

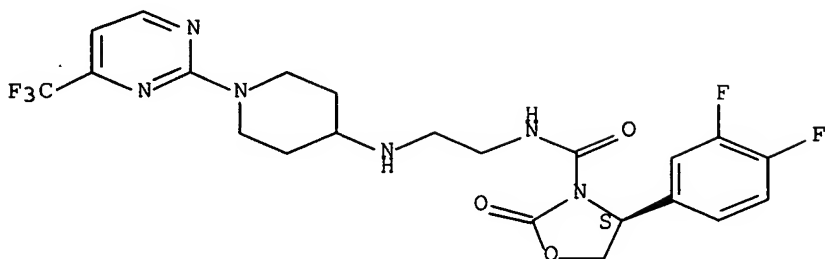
CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-1-[[[2-[[1-[3-(trifluoromethyl)-2-pyridinyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-, methyl ester, (6S)- (CA INDEX NAME)

Absolute stereochemistry.



INDEX NAME)

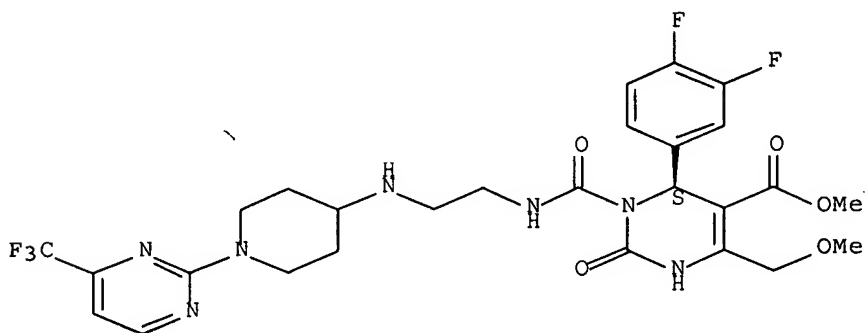
Absolute stereochemistry.



RN 218609-28-0 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-1-[[[2-[[1-(4-(trifluoromethyl)-2-pyrimidinyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-, methyl ester, (6S)- (CA INDEX NAME)

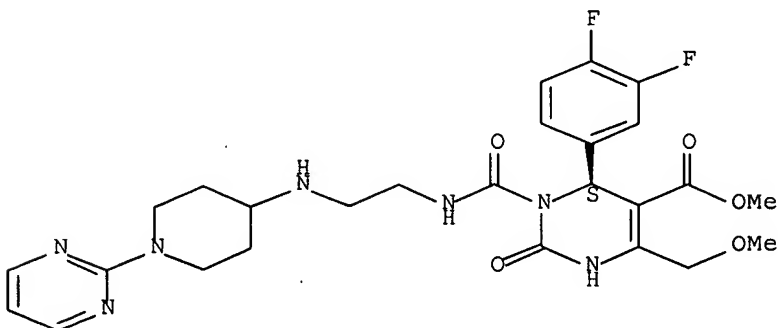
Absolute stereochemistry.

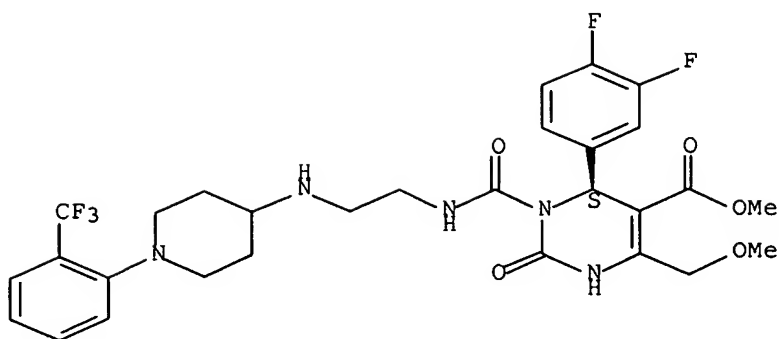


RN 218609-29-1 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-1-[[[2-[[1-(2-pyrimidinyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-, methyl ester, (6S)- (CA INDEX NAME)

Absolute stereochemistry.



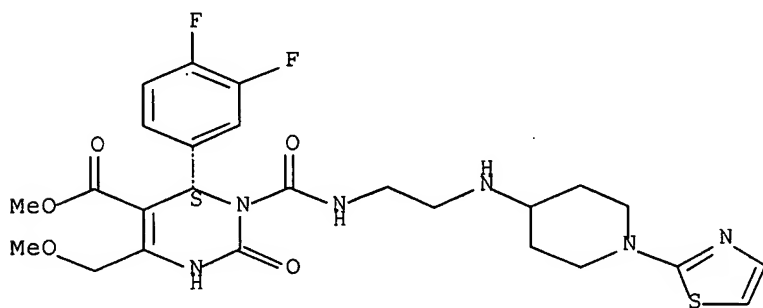


● HCl

RN 218609-33-7 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-1-[[[2-[[1-(2-thiazolyl)-4-piperidiny]amino]ethyl]amino]carbonyl]-, methyl ester, (6S)- (CA INDEX NAME)

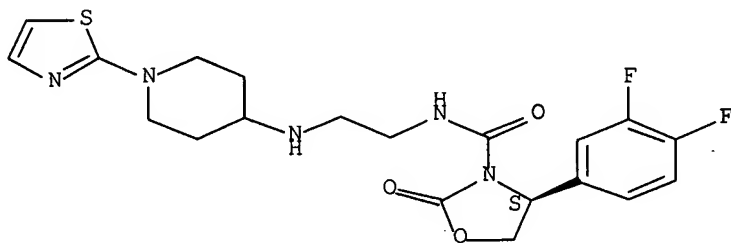
Absolute stereochemistry.



RN 218609-35-9 HCAPLUS

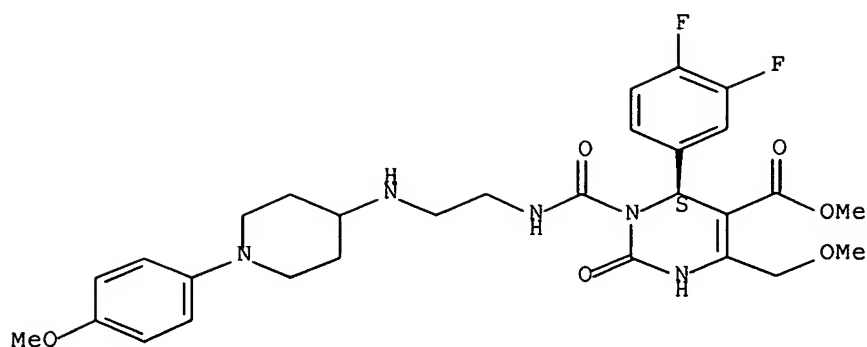
CN 3-Oxazolidinecarboxamide, 4-(3,4-difluorophenyl)-2-oxo-N-[2-[[1-(2-thiazolyl)-4-piperidiny]amino]ethyl]-, (4S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 218609-36-0 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-1-[[[2-[[1-(3-methyl-2-pyridinyl)-4-piperidiny]amino]ethyl]amino]carbonyl]-, methyl ester, (6S)- (CA INDEX NAME)

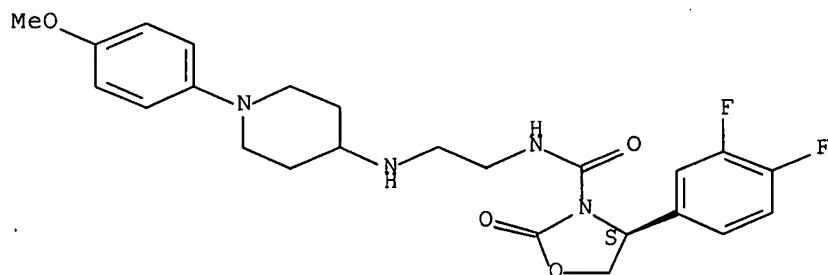


●2 HCl

RN 218609-40-6 HCAPLUS

CN 3-Oxazolidinecarboxamide, 4-(3,4-difluorophenyl)-N-[2-[[1-(4-methoxyphenyl)-4-piperidiny]amino]ethyl]-2-oxo-, dihydrochloride, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

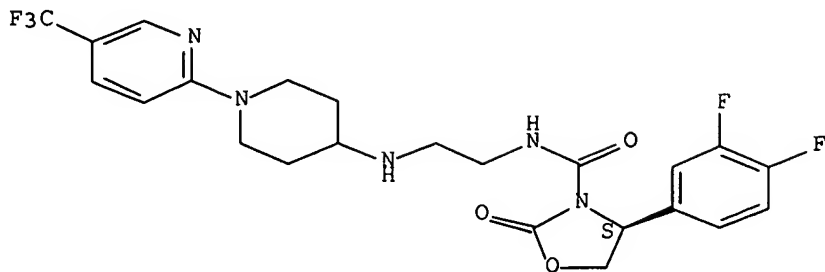
RN 218609-41-7 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-1-[[[2-[[1-(5-(trifluoromethyl)-2-pyridinyl]-4-piperidiny]amino]ethyl]amino]carbonyl]-, methyl ester, (6S)-(CA INDEX NAME)

Absolute stereochemistry.

INDEX NAME)

Absolute stereochemistry.



RN 218609-44-0 HCAPLUS

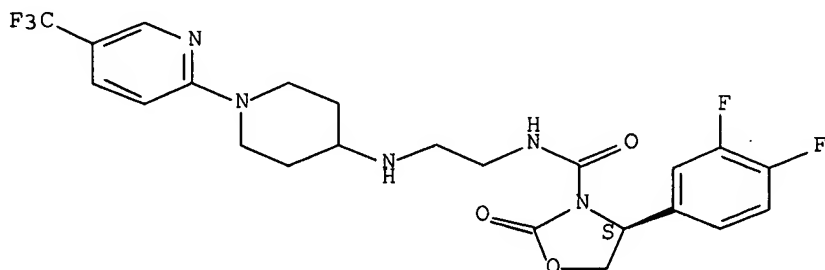
CN 3-Oxazolidinecarboxamide, 4-(3,4-difluorophenyl)-2-oxo-N-[2-[[1-[5-(trifluoromethyl)-2-pyridinyl]-4-piperidinyl]amino]ethyl]-, (4S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 218609-43-9

CMF C23 H24 F5 N5 O3

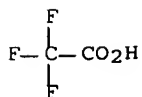
Absolute stereochemistry.



CM 2

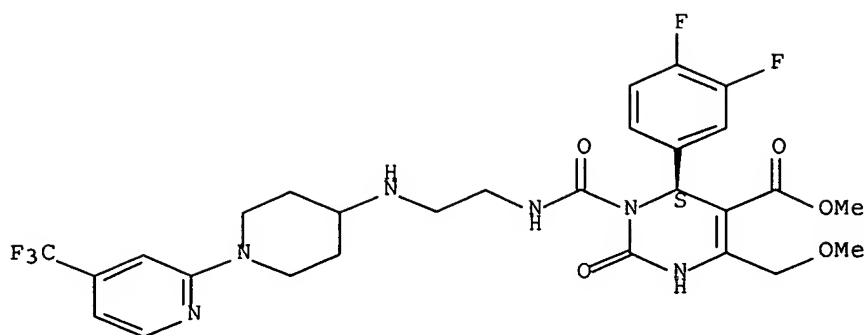
CRN 76-05-1

CMF C2 H F3 O2



RN 218609-45-1 HCAPLUS

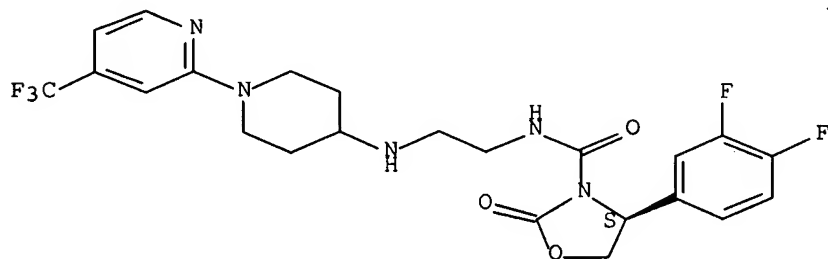
CN 3-Oxazolidinecarboxamide, 4-(3,4-difluorophenyl)-N-[2-[[1-(2,4-difluorophenyl)-4-piperidinyl]amino]ethyl]-2-oxo-, monohydrochloride, (4S)- (9CI) (CA INDEX NAME)



RN 218609-48-4 HCAPLUS

CN 3-Oxazolidinecarboxamide, 4-(3,4-difluorophenyl)-2-oxo-N-[2-[[1-[4-(trifluoromethyl)-2-pyridinyl]-4-piperidinyl]amino]ethyl]-, (4S)- (CA INDEX NAME)

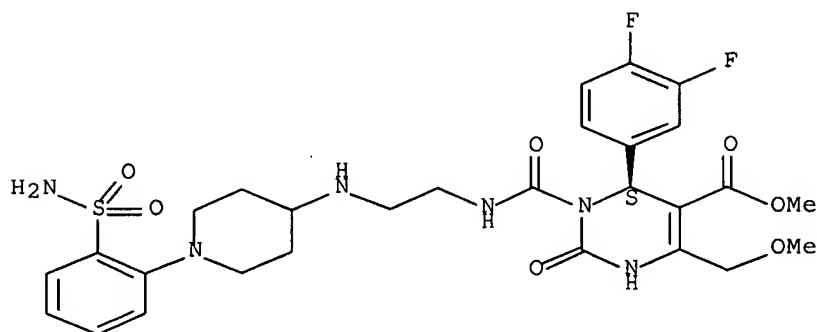
Absolute stereochemistry.



RN 218609-49-5 HCAPLUS

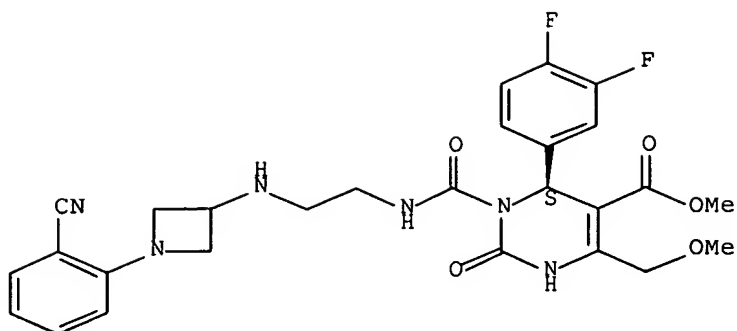
CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-[2-(aminosulfonyl)phenyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 218609-50-8 HCAPLUS

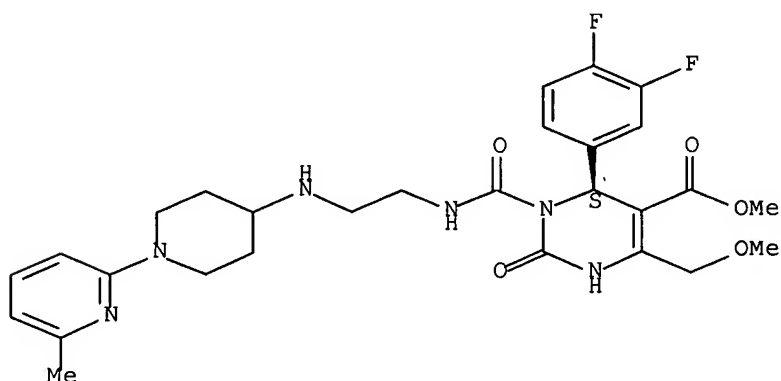
CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-1-[[[2-[[1-[2-(methylsulfonyl)phenyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-2-oxo-, methyl ester,



RN 218609-55-3 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-1-[[[2-[[1-(6-methyl-2-pyridinyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

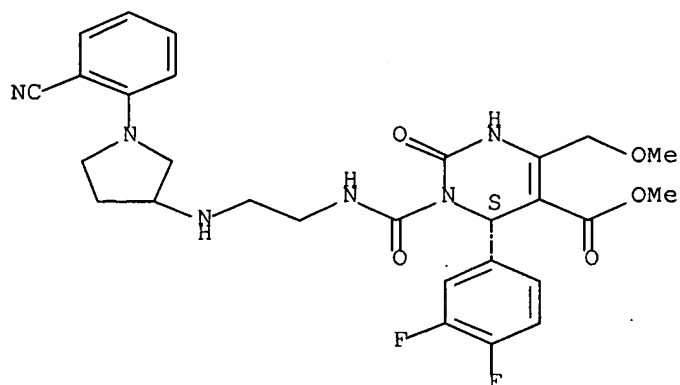
Absolute stereochemistry.

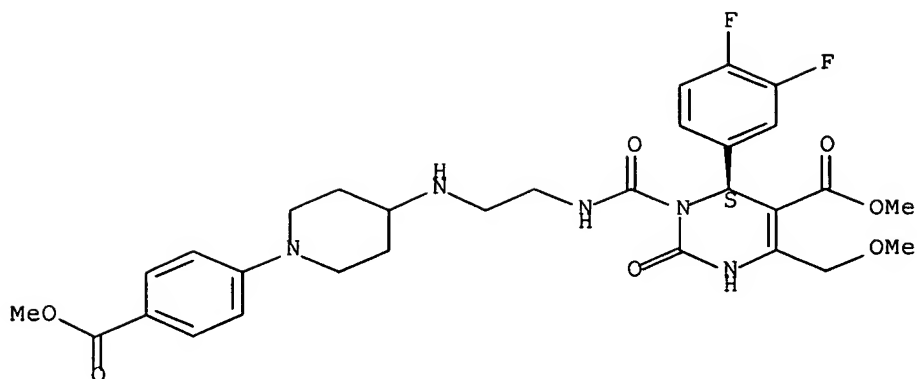


RN 218609-56-4 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-(2-cyanophenyl)-3-pyrrolidinyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

Absolute stereochemistry.

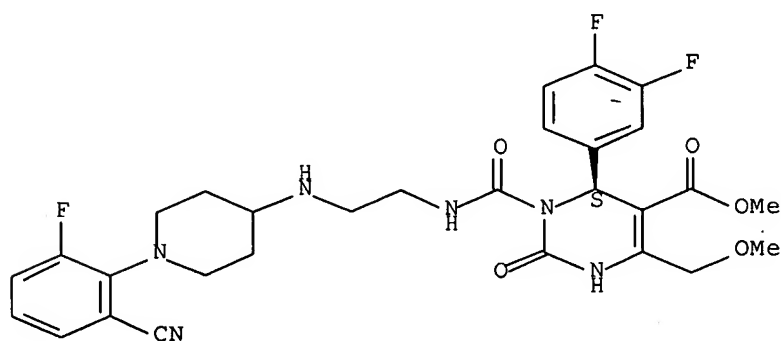




RN 218609-60-0 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-(2-cyano-6-fluorophenyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

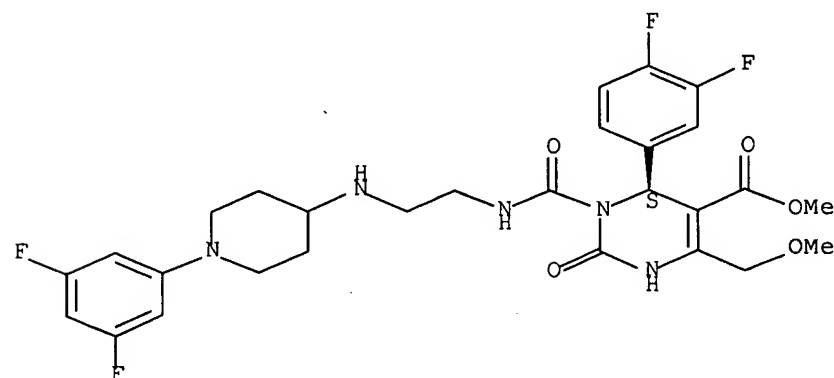
Absolute stereochemistry.



RN 218609-61-1 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1-[[[2-[[1-(3,5-difluorophenyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

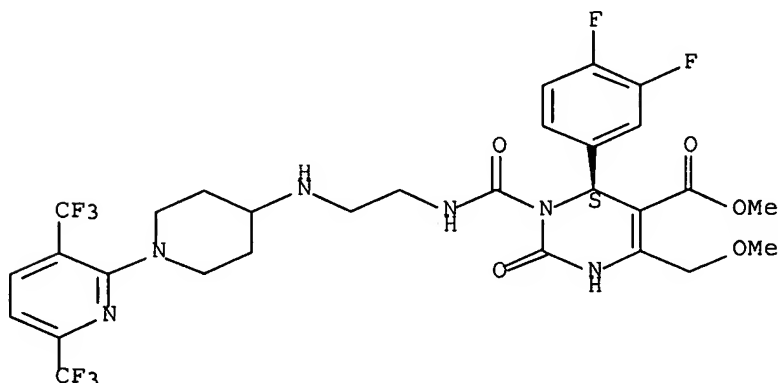
Absolute stereochemistry.



RN 218609-65-5 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-[3,6-bis(trifluoromethyl)-2-pyridinyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

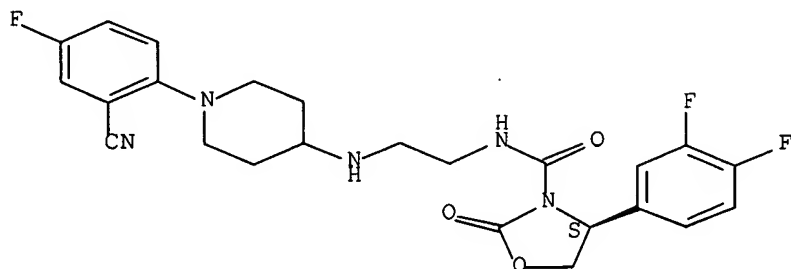
Absolute stereochemistry.



RN 218609-66-6 HCAPLUS

CN 3-Oxazolidinecarboxamide, N-[2-[[1-(2-cyano-4-fluorophenyl)-4-piperidinyl]amino]ethyl]-4-(3,4-difluorophenyl)-2-oxo-, (4S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 218609-67-7 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-[6-(acetylamino)-2-pyridinyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

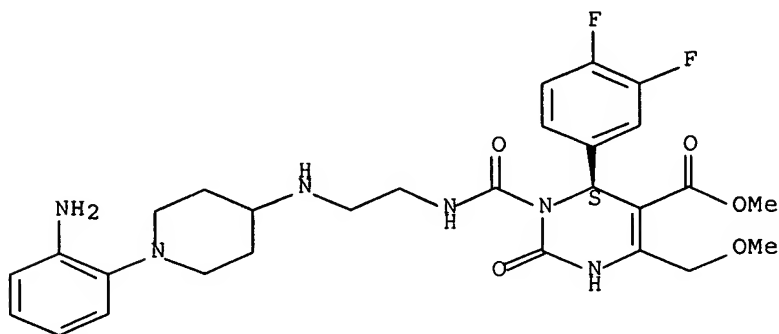
Absolute stereochemistry.



RN 218609-71-3 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-(2-aminophenyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

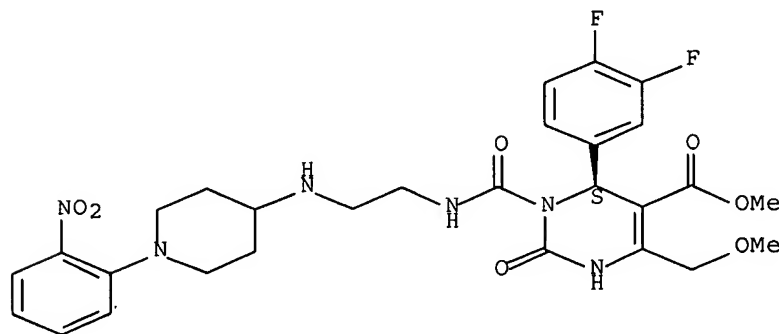
Absolute stereochemistry.



RN 218609-72-4 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-1-[[[2-[[1-(2-nitrophenyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

Absolute stereochemistry.

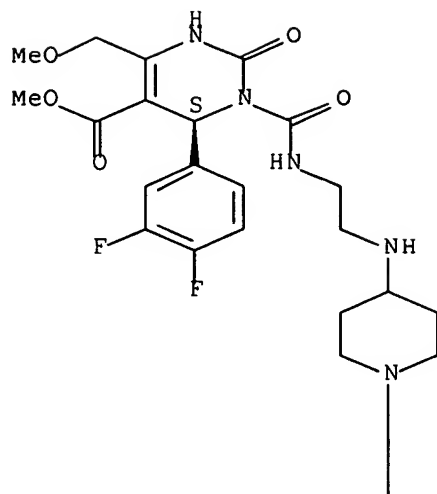


RN 218609-73-5 HCAPLUS

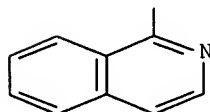
CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-[2-[(aminocarbonyl)amino]phenyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



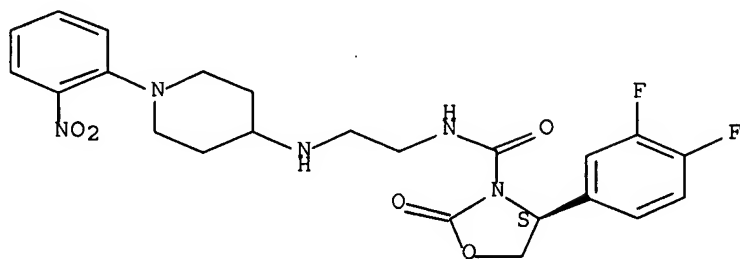
PAGE 2-A



RN 218609-76-8 HCAPLUS

CN 3-Oxazolidinecarboxamide, 4-(3,4-difluorophenyl)-N-[2-[[1-(2-nitrophenyl)-4-piperidinyl]amino]ethyl]-2-oxo-, (4S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 218609-77-9 HCAPLUS

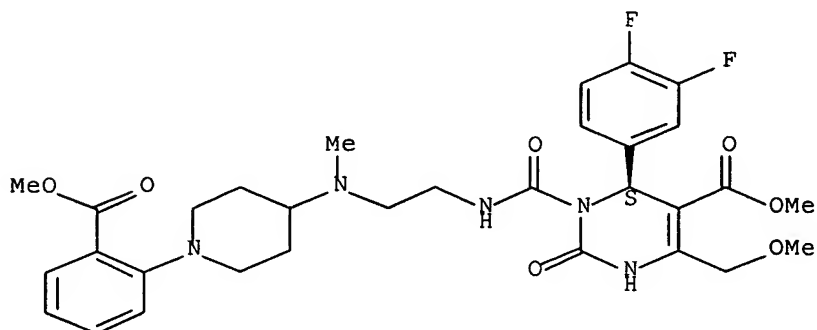
CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1-[[[2-[[1-(2-nitrophenyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 218609-80-4 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-1-  
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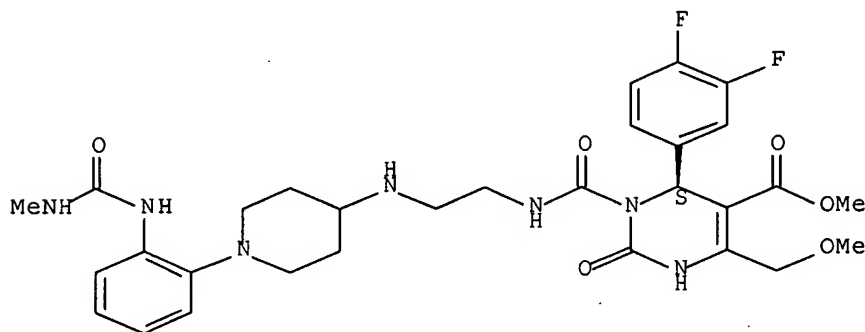
Absolute stereochemistry.



RN 218609-81-5 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-  
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 INDEX NAME)

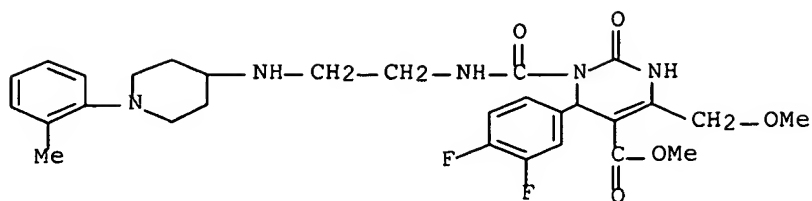
Absolute stereochemistry.



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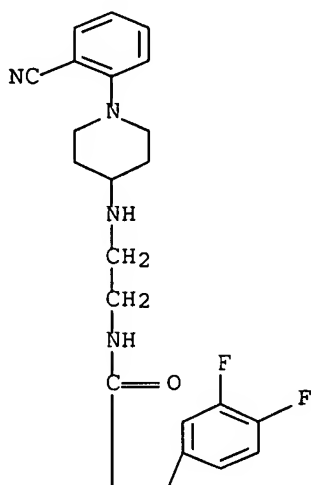
CN 3-Oxazolidinecarboxamide, 4-(3,4-difluorophenyl)-2-oxo-N-[2-[[1-(2-  
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Absolute stereochemistry.

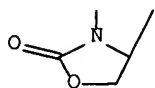


RN 218609-87-1 HCAPLUS  
 CN 3-Oxazolidinecarboxamide, N-[2-[[1-(2-cyanophenyl)-4-piperidinyl]amino]ethyl]-4-(3,4-difluorophenyl)-2-oxo- (CA INDEX NAME)

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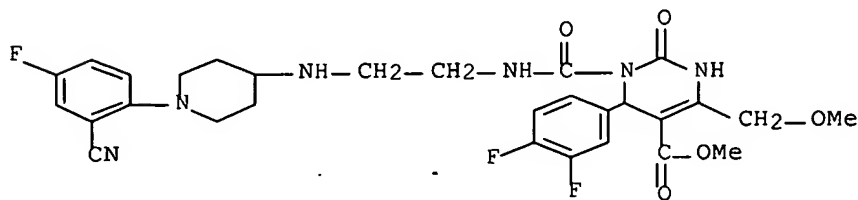
PAGE 2-A



RN 218609-89-3 HCAPLUS  
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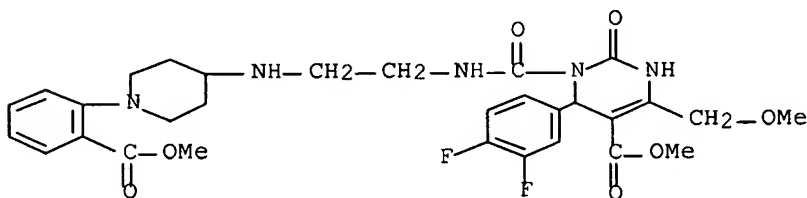
RN 218609-93-9 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-(2-cyano-4-fluorophenyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester (CA INDEX NAME)



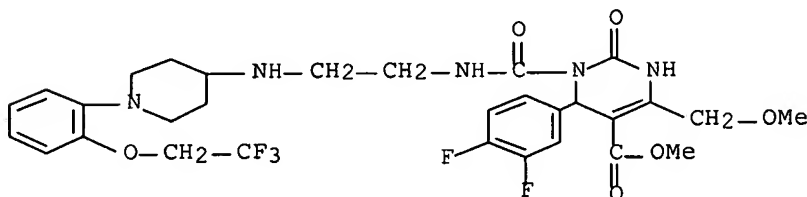
RN 218609-95-1 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-1-[[[2-[[1-[2-(methoxycarbonyl)phenyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-4-(methoxymethyl)-2-oxo-, methyl ester (CA INDEX NAME)



RN 218609-97-3 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-1-[[[2-[[1-[2-(2,2,2-trifluoroethoxy)phenyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

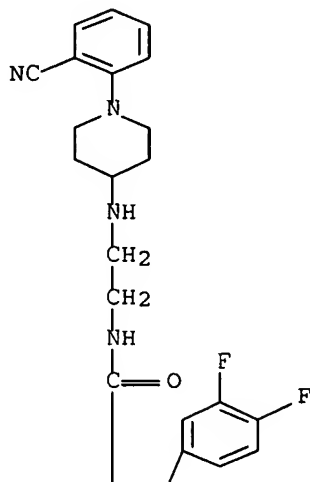


RN 218609-98-4 HCAPLUS

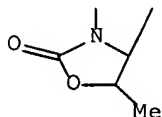
CN 3-Oxazolidinecarboxamide, 4-(3,4-difluorophenyl)-2-oxo-N-[2-[[1-[2-(2,2,2-trifluoroethoxy)phenyl]-4-piperidinyl]amino]ethyl]- (CA INDEX NAME)

RN 218610-04-9 HCAPLUS  
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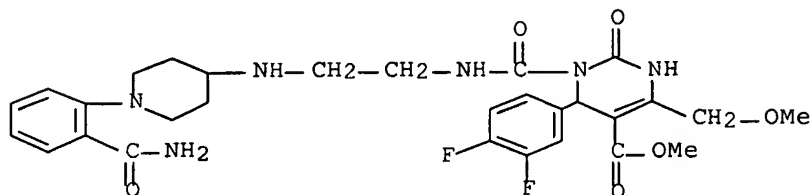
PAGE 1-A



PAGE 2-A

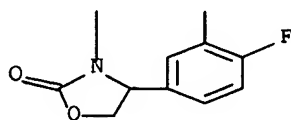


RN 218610-05-0 HCAPLUS  
 CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-[2-(aminocarbonyl)phenyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester (CA INDEX NAME)



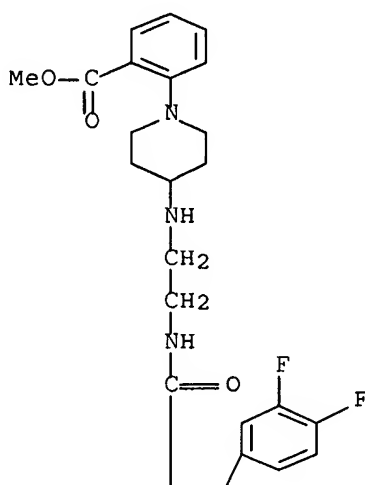
RN 218610-06-1 HCAPLUS  
 CN 3-Oxazolidinecarboxamide, N-[2-[[1-[2-(aminocarbonyl)phenyl]-4-piperidinyl]amino]ethyl]-4-(3,4-difluorophenyl)-2-oxo- (CA INDEX NAME)

PAGE 2-A

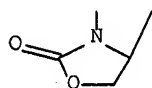


RN 218610-08-3 HCAPLUS  
 CN Benzoic acid, 2-[4-[[2-[[[4-(3,4-difluorophenyl)-2-oxo-3-oxazolidinyl]carbonyl]amino]ethyl]amino]-1-piperidinyl]-, methyl ester  
 (CA INDEX NAME)

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PAGE 2-A

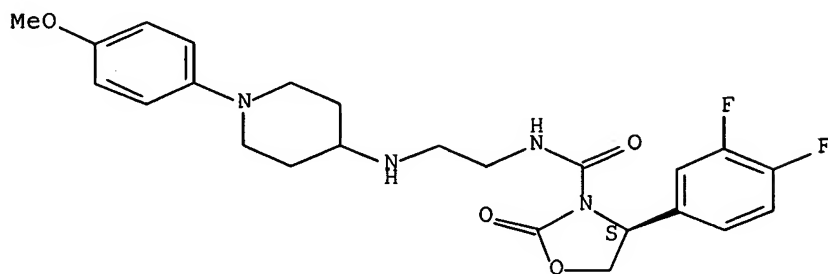


RN 218610-09-4 HCAPLUS  
 CN 3-Oxazolidinecarboxamide, 4-(3,4-difluorophenyl)-N-[2-[[1-(2-methoxyphenyl)-4-piperidinyl]amino]ethyl]-2-oxo-, (4S)- (CA INDEX NAME)

Absolute stereochemistry.

methoxyphenyl)-4-piperidiny]amino]ethyl]-2-oxo-, (4S)- (CA INDEX NAME)

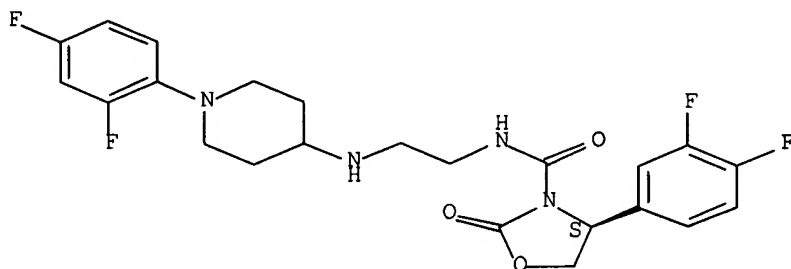
Absolute stereochemistry.



RN 218610-15-2 HCAPLUS

CN 3-Oxazolidinecarboxamide, 4-(3,4-difluorophenyl)-N-[2-[[1-(2,4-difluorophenyl)-4-piperidiny]amino]ethyl]-2-oxo-, (4S)- (CA INDEX NAME)

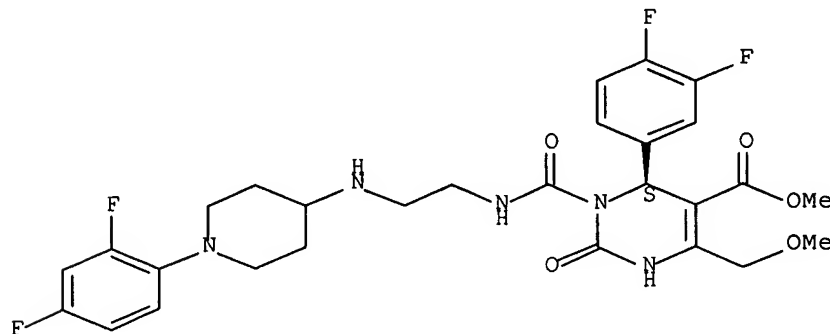
Absolute stereochemistry.



RN 218610-16-3 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1-[[[2-[[1-(2,4-difluorophenyl)-4-piperidiny]amino]ethyl]amino]carbonyl]-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

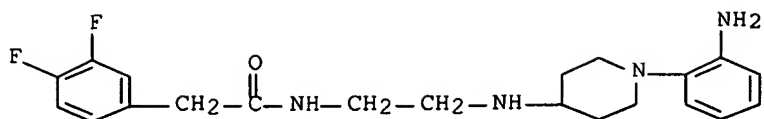
Absolute stereochemistry.



RN 218610-18-5 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-1-[[[2-[[1-(2-methylsulfonyl)phenyl]-4-piperidiny]amino]ethyl]amino]carbonyl]-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)





●3 HCl

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L167 ANSWER 15 OF 21 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:414235 HCAPLUS Full-text

DOCUMENT NUMBER: 129:172230

TITLE: Antibody catalysis of peptidyl-prolyl cis-trans isomerization in the folding of RNase T1

AUTHOR(S): Ma, Lifu; Hsieh-Wilson, Linda C.; Schultz, Peter G.

CORPORATE SOURCE: Howard Hughes Medical Institute, Department of Chemistry, University of California, Berkeley, CA, 94720, USA

SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1998), 95(13), 7251-7256

CODEN: PNASA6; ISSN: 0027-8424

PUBLISHER: National Academy of Sciences

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An antibody generated to an  $\alpha$ -keto amide containing hapten catalyzes the cis-trans isomerization of peptidyl-prolyl amide bonds in peptides and in the protein RNase T1. The antibody-catalyzed peptide isomerization reaction showed saturation kinetics for the cis-substrate, Suc-Ala-Ala-Pro-Phe- pNA, with a  $k_{cat}/K_m$  value of 883 s<sup>-1</sup>·M<sup>-1</sup>; the reaction was inhibited by a hapten analog ( $K_i = 3.0 \pm 0.4 \mu\text{M}$ ). Refolding of denatured RNase T1 to its native conformation also was catalyzed by the antibody, with the antibody-catalyzed folding reaction inhibitable both by the hapten and hapten analog. These results demonstrate that antibodies can catalyze conformational changes in protein structure, a transformation involved in many cellular processes.

CC 7-2 (Enzymes)

Section cross-reference(s): 27

IT 211385-93-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of a hapten that elicits an antibody capable of catalyzing peptidyl-prolyl cis-trans isomerization in the folding of RNase T1)

IT 75651-83-1P 174282-97-4P 211385-86-3P 211385-87-4P 211385-88-5P

211385-89-6P 211385-90-9P 211385-91-0P 211385-94-3P

211385-96-5P 211385-97-6P 211385-98-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of a hapten that elicits an antibody capable of catalyzing peptidyl-prolyl cis-trans isomerization in the folding of RNase T1)

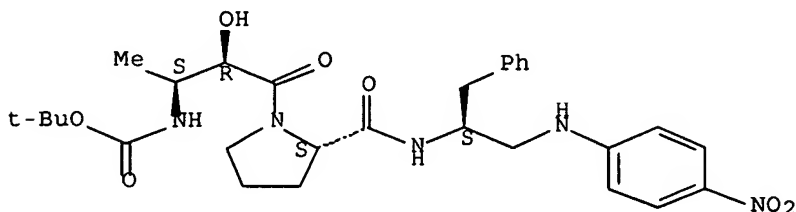
IT 211385-93-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of a hapten that elicits an antibody capable of catalyzing

nitrophenyl]amino]methyl]-2-phenylethyl]amino]carbonyl]-1-pyrrolidinyl]-3-oxopropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

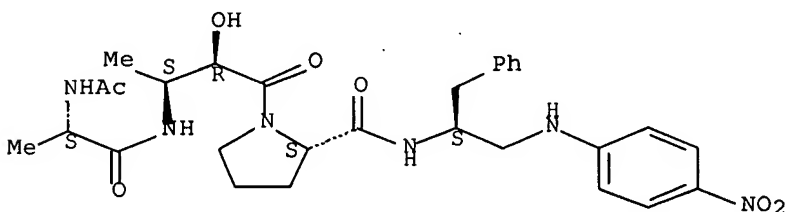
Absolute stereochemistry.



RN 211385-98-7 HCAPLUS

CN 2-Pyrrolidinecarboxamide, 1-[(2R,3S)-3-[[[(2S)-2-(acetamino)-1-oxopropyl]amino]-2-hydroxy-1-oxobutyl]-N-[(1S)-1-[[[4-nitrophenyl]amino]methyl]-2-phenylethyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L167 ANSWER 16 OF 21 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:239115 HCAPLUS Full-text

DOCUMENT NUMBER: 128:294793

TITLE: Preparation of benzodiazepines and dibenzo[a,d]cycloheptanes for stimulating bone formation

INVENTOR(S): Drake, Fred H.

PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA; Drake, Fred H.

SOURCE: PCT Int. Appl., 77 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9815278	A1	19980416	WO 1997-US18178	19971007 <--
W: JP, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 946180	A1	19991006	EP 1997-945563	19971007 <--
R: BE, CH, DE, ES, FR, GB, IT, LI, NL				
JP 2001501951	T	20010213	JP 1998-517727	19971007 <--
US 2002032187	A1	20020314	US 2001-956659	20010920 <--

175530-56-0P	175530-62-8P	175530-63-9P	175530-68-4P	175530-70-8P
175530-71-9P	175530-72-0P	175530-82-2P	175530-83-3P	175530-84-4P
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of benzodiazepines and dibenzo[a,d]cycloheptanes for stimulating bone formation)

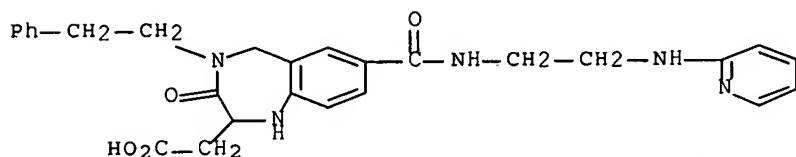
IT 193473-11-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzodiazepines and dibenzo[a,d]cycloheptanes for stimulating bone formation)

RN 193473-11-9 HCAPLUS

CN 1H-1,4-Benzodiazepine-2-acetic acid, 2,3,4,5-tetrahydro-3-oxo-4-(2-phenylethyl)-7-[[[2-(2-pyridinylamino)ethyl]amino]carbonyl]- (CA INDEX NAME)



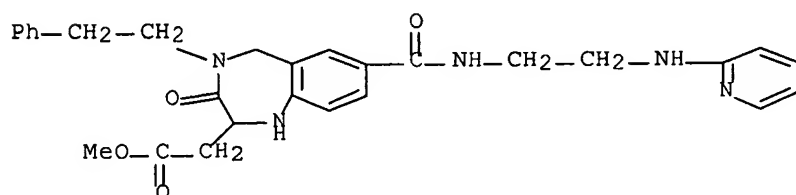
IT 193473-72-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of benzodiazepines and dibenzo[a,d]cycloheptanes for stimulating bone formation)

RN 193473-72-2 HCAPLUS

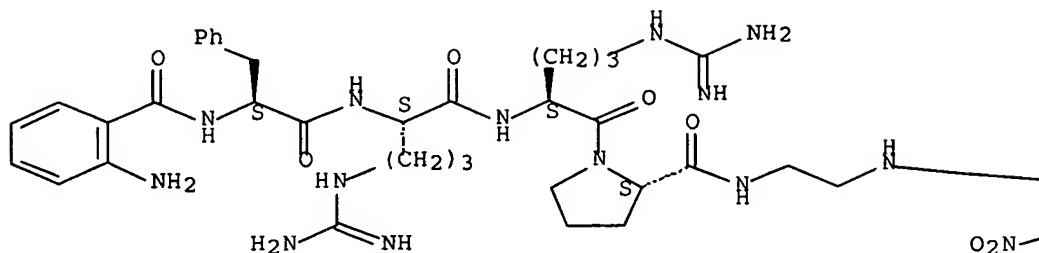
CN 1H-1,4-Benzodiazepine-2-acetic acid, 2,3,4,5-tetrahydro-3-oxo-4-(2-phenylethyl)-7-[[[2-(2-pyridinylamino)ethyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)



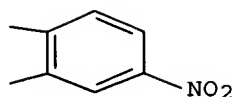
[(2,4-dinitrophenyl)amino]ethyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L167 ANSWER 18 OF 21 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1996:239755 HCAPLUS Full-text  
 DOCUMENT NUMBER: 124:289585  
 TITLE: Preparation of 3-oxo-2,3,4,5-tetrahydro-1H-1,4-benzodiazepine and -2-benzazepine derivatives and analogs as vitronectin receptor antagonists  
 INVENTOR(S): Cousins, Russell Donovan; Keenan, Richard Mcculloch; Kwon, Chet; Miller, William Henry; Uzinskas, Irene Nijole  
 PATENT ASSIGNEE(S): Smithkline Beecham Corp., USA  
 SOURCE: PCT Int. Appl., 55 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9600574	A1	19960111	WO 1995-US8146	19950629 <--
W: JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
ZA 9505391	A	19960209	ZA 1995-5391	19950629 <--
EP 762882	A1	19970319	EP 1995-925353	19950629 <--
R: BE, CH, DE, FR, GB, IT, NL				

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of oxotetrahydrobenzodiazepine and -benzazepine derivs. and analogs as vitronectin receptor antagonists)

IT 175531-31-4P 175532-99-7P 175533-00-3P 175533-01-4P 175533-02-5P  
 175533-03-6P 175533-04-7P 175533-05-8P 175533-07-0P 175533-08-1P  
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 175533-23-0P 175533-24-1P 175533-25-2P 175533-26-3P, Methyl

2-pyridylacetate hydrochloride 175672-23-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of oxotetrahydrobenzodiazepine and -benzazepine derivs. and analogs as vitronectin receptor antagonists)

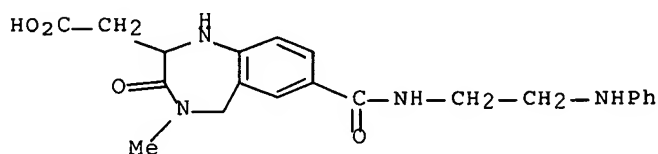
IT 175532-95-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of oxotetrahydrobenzodiazepine and -benzazepine derivs. and analogs as vitronectin receptor antagonists)

RN 175532-95-3 HCAPLUS

CN 1H-1,4-Benzodiazepine-2-acetic acid, 2,3,4,5-tetrahydro-4-methyl-3-oxo-7-[[[2-(phenylamino)ethyl]amino]carbonyl]- (CA INDEX NAME)



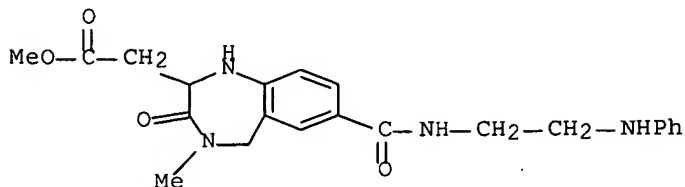
IT 175533-22-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of oxotetrahydrobenzodiazepine and -benzazepine derivs. and analogs as vitronectin receptor antagonists)

RN 175533-22-9 HCAPLUS

CN 1H-1,4-Benzodiazepine-2-acetic acid, 2,3,4,5-tetrahydro-4-methyl-3-oxo-7-[[[2-(phenylamino)ethyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)



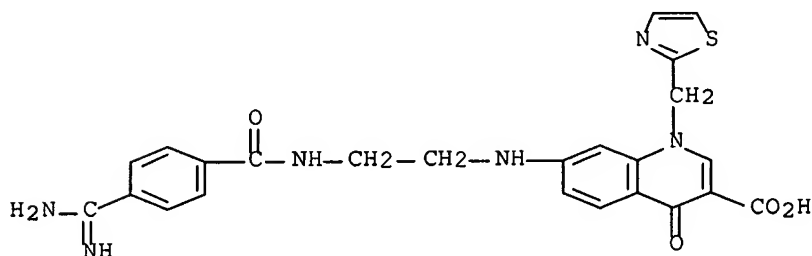
oxonaphthyridinecarboxylic acid derivs., their preparation, and their use  
as  
cell adhesion inhibitors)

IT 79660-72-3 94242-52-1 94242-53-2 99734-97-1 121859-55-0 124278-0  
6-4 125226-67-7 126052-17-3 127294-60-4 130436-09-8 137453-36-2  
158784-75-9 158784-76-0 158784-77-1 158784-78-2 158784-79-3  
158784-80-6 158784-81-7 158784-82-8 158784-83-9  
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158784-90-8 158784-91-9 158784-94-2 158784-95-3 158784-96-4  
158784-97-5 158784-98-6 158784-99-7 158785-00-3 158785-01-4  
158785-02-5 158785-03-6 158785-05-8 158785-06-9 158785-07-0  
158785-08-1 158785-09-2 158785-10-5 158785-11-6 158785-12-7  
158785-13-8 158785-14-9 158785-16-1 158785-17-2 158785-18-3  
158785-23-0 158850-79-4  
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(oxoquinolinecarboxylic acid derivs., oxonaphthyridinecarboxylic acid  
derivs., their preparation, and their use as cell adhesion inhibitors)

IT 158784-82-8  
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(oxoquinolinecarboxylic acid derivs., oxonaphthyridinecarboxylic acid  
derivs., their preparation, and their use as cell adhesion inhibitors)

RN 158784-82-8 HCAPLUS

CN 3-Quinolinecarboxylic acid, 7-[[2-[[4-(aminoiminomethyl)benzoyl]amino]ethy  
l]amino]-1,4-dihydro-4-oxo-1-(2-thiazolylmethyl)- (CA INDEX NAME)



L167 ANSWER 20 OF 21 HCAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1983:125577 HCAPLUS Full-text  
DOCUMENT NUMBER: 98:125577  
ORIGINAL REFERENCE NO.: 98:19119a,19122a  
TITLE: On the antimicrobial activity and syntheses of  
carbanilide and salicylanilide derivatives  
AUTHOR(S): Takeuchi, Isao; Yamamoto, Kazuko; Hamada, Yoshiki;  
Ito, Tomiyoshi  
CORPORATE SOURCE: Fac. Pharm., Meijo Univ., Nagoya, 468, Japan  
SOURCE: Yakugaku Zasshi (1982), 102(11), 1023-30  
CODEN: YKKZAJ; ISSN: 0031-6903  
DOCUMENT TYPE: Journal  
LANGUAGE: Japanese  
OTHER SOURCE(S): CASREACT 98:125577  
GI

CODEN: ARZNAD; ISSN: 0004-4172

DOCUMENT TYPE: Journal

LANGUAGE: German

AB One hundred eighty different Ph substituted thioureas (R1NHCSNH r2) were tested for tuberculostatic activity in vitro and in the mouse. The tables presented indicate that p-BuOC6H4NHCSNHC6H4OBu-m (I) had the greatest activity in vitro (0.1-0.2 µg/ml) while in vivo I was most active at a dosage of 250 mg/kg body weight when given orally.

CC 15 (Pharmacodynamics)

IT 92-96-6 27070-87-7 27677-70-9 27677-71-0 27677-72-1 27677-73-2  
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 27828-69-9 27828-70-2

RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); THU (Therapeutic use); BIOL  
 (Biological study); USES (Uses)  
 (antitubercular activity of)

IT 27683-15-4

RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); THU (Therapeutic use); BIOL  
 (Biological study); USES (Uses)  
 (antitubercular activity of)

RN 27683-15-4 HCAPLUS

CN Carbanilide, 4-butoxy-4'-(p-chloroanilino)thio- (8CI) (CA INDEX NAME)

## TEXT SEARCH

=> fil hcapl; d que l162

FILE 'HCAPLUS' ENTERED AT 15:54:01 ON 30 JAN 2008

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FILE COVERS 1907 - 30 Jan 2008 VOL 148 ISS 5

FILE LAST UPDATED: 29 Jan 2008 (20080129/ED)

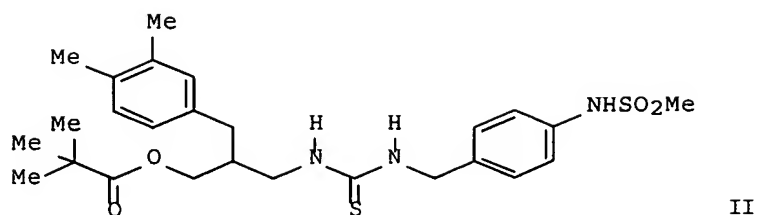
New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

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L14	1695	SEA	FILE=HCAPLUS	ABB=ON	NEURALGI?/OBI
L15	146	SEA	FILE=HCAPLUS	ABB=ON	CAUSALGI?/OBI
L16	355	SEA	FILE=HCAPLUS	ABB=ON	POLYNEURITIS/OBI
L17	32	SEA	FILE=HCAPLUS	ABB=ON	NEURONITIS/OBI
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L19	198	SEA	FILE=HCAPLUS	ABB=ON	TOOTHACHE/OBI OR TOOTH/OBI(L)ACHE/OBI
L20	1574	SEA	FILE=HCAPLUS	ABB=ON	BITE#/OBI OR STING#/OBI
L21	214	SEA	FILE=HCAPLUS	ABB=ON	SYMPATHETIC/OBI(L)DYSTROPH?/OBI
L22	39283	SEA	FILE=HCAPLUS	ABB=ON	ARTHRITIS/OBI
L23	1155	SEA	FILE=HCAPLUS	ABB=ON	FIBROMYALGIA/OBI
L24	2	SEA	FILE=HCAPLUS	ABB=ON	GUILLIAN BARRE/OBI
L25	32	SEA	FILE=HCAPLUS	ABB=ON	PARESTHETICA/OBI(L)MERALGI?/OBI
L26	50	SEA	FILE=HCAPLUS	ABB=ON	BURNING MOUTH/OBI
L27	7354	SEA	FILE=HCAPLUS	ABB=ON	HEADACHE/OBI OR HEAD/OBI(L)ACHE/OBI
L28	284	SEA	FILE=HCAPLUS	ABB=ON	CHILDBIRTH/OBI
L29	6567	SEA	FILE=HCAPLUS	ABB=ON	MENSTRUUA?/OBI
L30	9	SEA	FILE=HCAPLUS	ABB=ON	LABOR/OBI(L)OBSTETRIC/OBI
L31	1419	SEA	FILE=HCAPLUS	ABB=ON	GUILLAIN BARRE/OBI
L32	416	SEA	FILE=HCAPLUS	ABB=ON	CAPSAICIN RECEPTORS/CT(L) (ANTAG?/OBI OR INHIB?/OBI OR BLOCK?/OBI)
L33	12049	SEA	FILE=HCAPLUS	ABB=ON	PARTURITION/CT
L34	58509	SEA	FILE=HCAPLUS	ABB=ON	ANALGES?/OBI
L161	20	SEA	FILE=HCAPLUS	ABB=ON	L32 AND (PY<2001 OR AY<2001 OR PRY<2001)
L162	10	SEA	FILE=HCAPLUS	ABB=ON	L161 AND (L12 OR L13 OR L14 OR L15 OR L16 OR L17 OR L18 OR L19 OR L20 OR L21 OR L22 OR L23 OR L24 OR L25 OR L26 OR L27 OR L28 OR L29 OR L30 OR L31 OR L33 OR L34)





AB RNHC(:X)ZZ1NHR1 [I; e.g., R = R4CO2CH2CH(CH2R5)CH2 and Z = NHCH2; R1 = alkylsulfonyl, arylsulfonyl, alkanoyl, etc.; Z1 = (3-halo- or -methoxy) 1,4-phenylene; X = O or S] were prepared. Thus, title compound II was prepared. Data for biol. activity of I were given.

IC ICM C07C335-16

ICS A61K031-222

CC 25-21 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
Section cross-reference(s): 1

ST acylaminophenylthiourea prepn vanilloid receptor antagonist;  
analgesic acylaminophenylthiourea prepn; antiinflammatory  
acylaminophenylthiourea prepn

IT Analgesics

Anti-inflammatory agents

(preparation of N-(acylaminophenyl)thioureas as vanilloid receptor antagonists)

IT Capsaicin receptors

RL: BSU (Biological study, unclassified); BIOL (Biological study)

(preparation of N-(acylaminophenyl)thioureas as vanilloid receptor antagonists)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L168 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:157732 HCAPLUS Full-text

DOCUMENT NUMBER: 136:216540

TITLE: Preparation of novel thiocarbamic acid derivatives as vanilloid receptor antagonists

INVENTOR(S): Suh, Young Ger; Oh, Uh Taek; Kim, Hee Doo; Lee, Jee Woo; Park, Hyeung Geun; Park, Young Ho; Yi, Jung Bum

PATENT ASSIGNEE(S): Pacific Corporation, S. Korea

SOURCE: PCT Int. Appl., 102 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002016317	A1	20020228	WO 2001-KR1409	20010820 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,				

IT Analgesics  
 Anti-inflammatory agents  
 Antiasthmatics  
 Antimigraine agents  
 Antiulcer agents  
 Human  
 (preparation of novel thiocarbamic acid derivs. as vanilloid receptor antagonists)

IT Capsaicin receptors  
 RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 (preparation of novel thiocarbamic acid derivs. as vanilloid receptor antagonists)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L168 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:635917 HCAPLUS Full-text

DOCUMENT NUMBER: 134:428

TITLE: Arginine-rich peptides are blockers of VR-1 channels with analgesic activity

AUTHOR(S): Planells-Cases, R.; Aracil, A.; Merino, J. M.; Gallar, J.; Perez-Paya, E.; Belmonte, C.; Gonzalez-Ros, J. M.; Ferrer-Montiel, A. V.

CORPORATE SOURCE: Centro de Biologia Molecular y Celular, Edf. Torregaitan, Avda. Ferrocarril s/n, Universidad Miguel Hernandez, Elche (Alicante), 03202, Spain

SOURCE: FEBS Letters (2000), 481(2), 131-136

CODEN: FEBLAL; ISSN: 0014-5793

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Vanilloid receptors (VRs) play a fundamental role in the transduction of peripheral tissue injury and/or inflammation responses. Mols. that antagonize VR channel activity may act as selective and potent analgesics. We report that synthetic arginine-rich hexapeptides block heterologously expressed VR-1 channels with submicromolar efficacy in a weak voltage-dependent manner, consistent with a binding site located near/at the entryway of the aqueous pore. Dynorphins, natural arginine-rich peptides, also blocked VR-1 activity with micromolar affinity. Notably, synthetic and natural arginine-rich peptides attenuated the ocular irritation produced by topical capsaicin application onto the eyes of exptl. animals. Taken together, our results imply that arginine-rich peptides are VR-1 channel blockers with analgesic activity. These findings may expand the development of novel analgesics by targeting receptor sites distinct from the capsaicin binding site.

CC 1-11 (Pharmacology)

ST vanilloid receptor arginine rich peptide analgesic

IT Analgesics

(arginine-rich peptides are blockers of VR-1 channels)

IT Capsaicin receptors

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(arginine-rich peptides are blockers of VR-1 channels)

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L168 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:510255 HCAPLUS Full-text

DOCUMENT NUMBER: 131:295096

TITLE: Unsaturated Long-Chain N-Acyl-vanillyl-amides (N-AVAMS): Vanilloid Receptor Ligands That Inhibit

SOURCE: Anesthesiology (1999), 90(2), 524-534  
CODEN: ANESAV; ISSN: 0003-3022  
PUBLISHER: Lippincott Williams & Wilkins  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Background: Capsaicin, the pungent ingredient in chili peppers, is a vanilloid with noxious and analgesic effects that inhibits tetrodotoxin-resistant sodium currents. Because tetrodotoxin-resistant currents are found primarily in small-diameter nociceptor afferents of the peripheral nerves, their inhibition may lead to selective analgesia. Therefore, the authors evaluated the interactions between tetrodotoxin, a site 1 sodium channel blocker, and capsaicin on nerve blockade in vivo. Methods: Percutaneous sciatic nerve injections with 0 to 9.9 mM capsaicin, 0 to 120  $\mu$ M tetrodotoxin, or both were administered to male Sprague-Dawley rats. Thermal nociceptive and motor blockade were measured. Data were expressed as medians with 25th and 75th percentiles. Results: Capsaicin produced a transient increase in thermal latency with no effect on motor strength. Tetrodotoxin reduced motor strength for a longer duration than nociception. The interaction between tetrodotoxin and capsaicin was synergistic, as evidenced by (1) supraadditive prolongation of both nociceptive and motor block, with the effect of capsaicin reversed by the vanilloid antagonist capsazepine, and (2) synergism in the frequency that rats achieved maximal block shown by isobolog. anal. The combination of tetrodotoxin and capsaicin showed less motor predominance than tetrodotoxin did alone. Similar interactions were found between tetrodotoxin and resiniferatoxin (another vanilloid), and between capsaicin and saxitoxin (another site 1 sodium channel blocker), but much less so between bupivacaine and capsaicin. Conclusions: Site 1 sodium channel blockers and vanilloids have synergistic effects on nerve blockade in vivo. These interactions may be useful in developing prolonged local anesthetics and elucidating mechanisms of functionally selective nerve blockade.

CC 1-11 (Pharmacology)

IT Analgesics

(vanilloid receptor agonists potentiate local anesthetic activity of percutaneously injected site 1 sodium channel blockers)

IT Capsaicin receptors

RL: BSU (Biological study, unclassified); BIOL (Biological study)

(vanilloid receptor agonists potentiate local anesthetic activity of percutaneously injected site 1 sodium channel blockers)

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L168 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:34840 HCAPLUS Full-text

DOCUMENT NUMBER: 130:105328

TITLE: Use of antagonists or partial agonists of the vanilloid receptor complexes for treating neurodegenerative diseases

INVENTOR(S): Benham, Christopher David; Davis, John; Parsons, Andrew

PATENT ASSIGNEE(S): Smithkline Beecham Plc, UK

SOURCE: PCT Int. Appl., 15 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
WO 9900115	A1	19990107	WO 1998-EP4005	19980618 <--

IT Capsaicin receptors

RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(anandamide transport inhibition by vanilloid agonist  
olvanil)

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L168 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:435382 HCAPLUS Full-text

DOCUMENT NUMBER: 129:131036

TITLE: A capsaicin-receptor antagonist, capsazepine, reduces  
inflammation-induced hyperalgesic responses in the  
rat: evidence for an endogenous capsaicin-like  
substance

AUTHOR(S): Kwak, J. Y.; Jung, J. Y.; Hwang, S. W.; Lee, W. T.;  
Oh, U.

CORPORATE SOURCE: The Sensory Research Group, College of Pharmacy,  
Creative Research Initiative Program, Seoul National  
University, Seoul, 151-742, S. Korea

SOURCE: Neuroscience (Oxford) (1998), 86(2), 619-626  
CODEN: NRSCDN; ISSN: 0306-4522

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The presence of an endogenous capsaicin-like substance and the role of  
capsaicin receptors in nociception during inflammation were assessed using Fos  
immunohistochem. and the paw withdrawal test in rats. Intradermal injection  
of carrageenan in the hindpaw produced inflammation in the foot pad, increased  
the number of cells exhibiting Fos-like immunoreactivity in the dorsal horn of  
the spinal cord, and decreased the paw withdrawal latency. Intradermal  
injection of capsazepine reduced the number of cells with the Fos-like  
immunoreactivity and increased the paw withdrawal latency, but did not  
decrease the inflammation induced by carrageenan. Intradermal injection of  
capsaicin or formalin also increased the Fos-pos. neuron number Capsaicin- or  
formalin-induced Fos expression was decreased in both cases by pretreatment  
with capsazepine, but to a much lesser extent for formalin. The capsazepine  
inhibition of carrageenan inflammation-induced hyperalgesic responses strongly  
suggests that an endogenous capsaicin-like substance is released in inflamed  
tissues and produces nociceptive neural impulses by acting on capsaicin  
receptors present on sensory neurons. Capsaicin receptors may take part only  
in generating nociceptive signals in sensory neurons, but not in activating  
the inflammation-promoting cells.

CC 1-7 (Pharmacology)

Section cross-reference(s): 14

ST capsazepine capsaicin receptor inflammation analgesia; capsaicin  
like substance inflammation analgesia capsazepine

IT Analgesia

Inflammation

(capsazepine capsaicin receptor antagonist reduces inflammation-induced  
hyperalgesia in rats and role of endogenous capsaicin-like substance)

IT Capsaicin receptors

Capsaicinoids

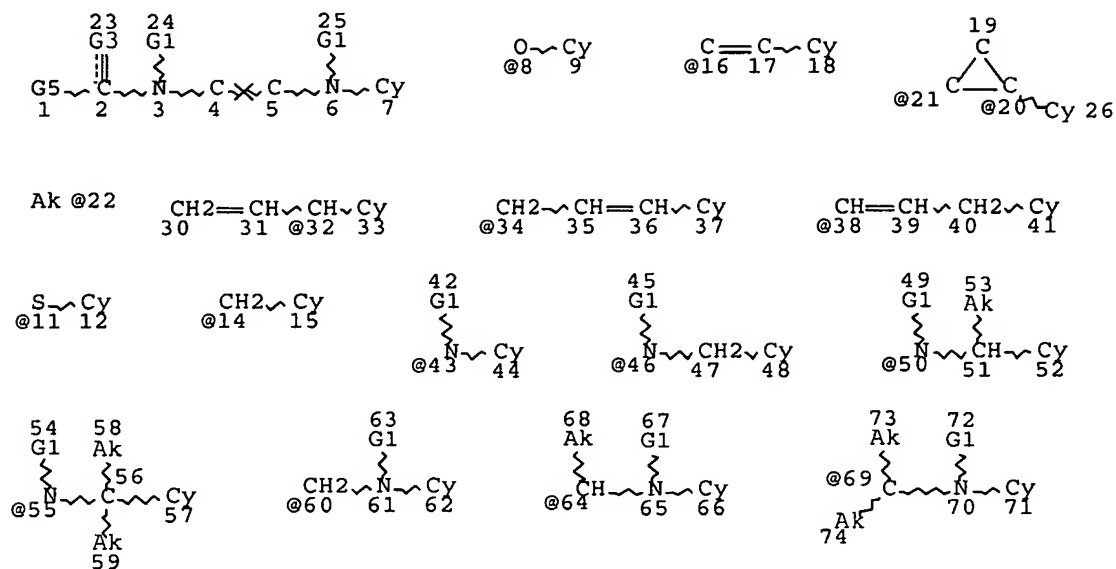
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL  
(Biological study); PROC (Process)

(capsazepine capsaicin receptor antagonist reduces  
inflammation-induced hyperalgesia in rats and role of endogenous  
capsaicin-like substance)

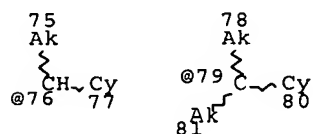
REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS  
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## SEARCH HISTORY

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L42          SCR 1839 AND 1993
L50          STR
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Page 1-A



Page 2-A

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VAR G3=0/S

VAR G5=CY/8/11/14/16/20/21/32/34/38/43/46/50/55/60/64/69/14/76/79

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NSPEC IS RC AT 5

CONNECT IS E1 RC AT 22

CONNECT IS E1 RC AT 53

CONNECT IS E1 RC AT 58

CONNECT IS E1 RC AT 59

CONNECT IS E1 RC AT 68

CONNECT IS E1 RC AT .73

CONNECT IS E1 RC AT 74

CONNECT IS E1 RC AT 75

CONNECT IS E1 RC AT 78

CONNECT IS E1 RC AT 81

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DEFAULT ECLEVEL IS LIMITED

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DEFAULT ECLEVEL IS LIMITED

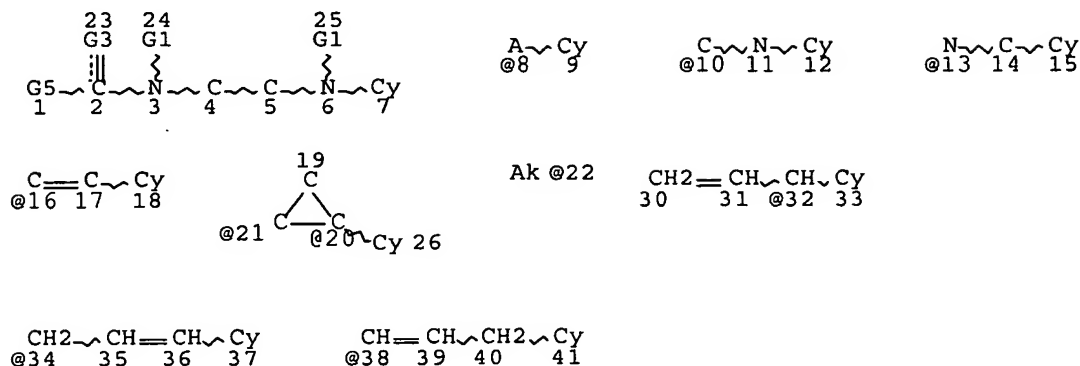
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NUMBER OF NODES IS 39

STEREO ATTRIBUTES: NONE

L89 STR



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VAR G3=O/S

VAR G5=CY/8/10/13/16/21/20/32/34/38

NODE ATTRIBUTES:

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NSPEC IS R AT 5

CONNECT IS E1 RC AT 22

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

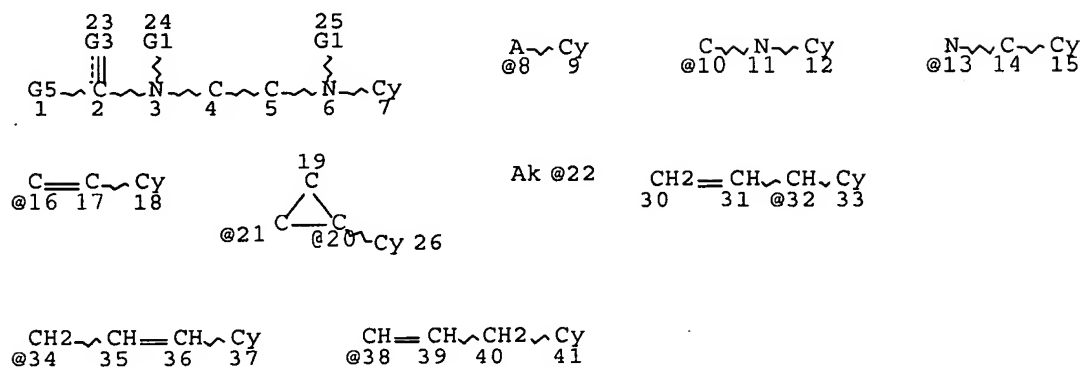
GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 38

STEREO ATTRIBUTES: NONE

L90 STR



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VAR G3=O/S

VAR G5=CY/8/10/13/16/21/20/32/34/38

NODE ATTRIBUTES:

-0/BI OR 393514-71-1/BI OR 393514-72-2/BI OR 393514-73-3/BI OR  
 393514-74-4/BI OR 393514-75-5/BI OR 393514-76-6/BI OR 393514-77  
 -7/BI OR 393514-78-8/BI OR 393514-79-9/BI OR 393514-80-2/BI OR  
 393514-81-3/BI OR 393514-82-4/BI OR 393514-83-5/BI OR 393514-84  
 -6/BI OR 393514-85-7/BI OR 393514-86-8/BI OR 393514-87-9/BI OR  
 393514-88-0/BI OR 393514-89-1/BI OR 393514-90-4/BI OR 393514-91  
 -5/BI OR 393514-92-6/BI OR

L3 STR  
 L4 50 SEA SSS SAM L3

FILE 'ZCAPLUS' ENTERED AT 12:01:04 ON 30 JAN 2008  
 D SCAN L1

FILE 'REGISTRY' ENTERED AT 12:01:05 ON 30 JAN 2008

FILE 'STNGUIDE' ENTERED AT 12:02:01 ON 30 JAN 2008

FILE 'HCAPLUS' ENTERED AT 12:11:12 ON 30 JAN 2008

L5 1 SEA ABB=ON US2004-799286/APPS  
 L6 63 SEA ABB=ON BAKTHAVATCHALAM R?/AU  
 L7 235 SEA ABB=ON HUTCHISON A?/AU  
 L8 103 SEA ABB=ON DESIMONE R?/AU  
 L9 55 SEA ABB=ON HODGETTS K?/AU  
 L10 1056 SEA ABB=ON KRAUSE J?/AU  
 L11 2037 SEA ABB=ON WHITE G?/AU  
 L12 13783 SEA ABB=ON NEUROPATH?/OBI  
 L13 1523 SEA ABB=ON NEURITIS/OBI  
 L14 1695 SEA ABB=ON NEURALGI?/OBI  
 L15 146 SEA ABB=ON CAUSALGI?/OBI  
 L16 355 SEA ABB=ON POLYNEURITIS/OBI  
 L17 32 SEA ABB=ON NEURONITIS/OBI  
 L18 25102 SEA ABB=ON PAIN/CT  
 L19 198 SEA ABB=ON TOOTHACHE/OBI OR TOOTH/OBI (L)ACHE/OBI  
 L20 1574 SEA ABB=ON BITE#/OBI OR STING#/OBI  
 L21 214 SEA ABB=ON SYMPATHETIC/OBI (L)DYSTROPH?/OBI  
 L22 39283 SEA ABB=ON ARTHRITIS/OBI  
 L23 1155 SEA ABB=ON FIBROMYALGIA/OBI  
 L24 2 SEA ABB=ON GUILLIAN BARRE/OBI  
 L25 32 SEA ABB=ON PARESTHETICA/OBI (L)MERALGI?/OBI  
 L26 50 SEA ABB=ON BURNING MOUTH/OBI  
 L27 7354 SEA ABB=ON HEADACHE/OBI OR HEAD/OBI (L)ACHE/OBI  
 L28 284 SEA ABB=ON CHILDBIRTH/OBI  
 L29 6567 SEA ABB=ON MENSTRUA?/OBI  
 L30 9 SEA ABB=ON LABOR/OBI (L)OBSTETRIC/OBI  
 L31 1419 SEA ABB=ON GUILLAIN BARRE/OBI  
 L32 416 SEA ABB=ON CAPSAICIN RECEPTORS/CT (L) (ANTAG?/OBI OR INHIB?/OBI  
 OR BLOCK?/OBI)  
 L33 12049 SEA ABB=ON PARTURITION/CT  
 D SCAN L5  
 L34 58509 SEA ABB=ON ANALGES?/OBI

FILE 'STNGUIDE' ENTERED AT 12:14:22 ON 30 JAN 2008

FILE 'HCAPLUS' ENTERED AT 12:16:48 ON 30 JAN 2008

L35 146669 SEA ABB=ON (L5 OR L6 OR L7 OR L8 OR L9 OR L10 OR L11 OR L12  
 OR L13 OR L14 OR L15 OR L16 OR L17 OR L18 OR L19 OR L20 OR L21  
 OR L22 OR L23 OR L24 OR L25 OR L26 OR L27 OR L28 OR L29 OR L30  
 OR L31 OR L32 OR L33 OR L34)

FILE 'REGISTRY' ENTERED AT 12:17:32 ON 30 JAN 2008

FILE 'STNGUIDE' ENTERED AT 14:51:03 ON 30 JAN 2008

FILE 'LREGISTRY' ENTERED AT 14:51:49 ON 30 JAN 2008

L55 SCREEN 2041  
L56 STR  
L57 50 SEA SSS SAM L56 AND L55

FILE 'STNGUIDE' ENTERED AT 14:52:55 ON 30 JAN 2008

FILE 'REGISTRY' ENTERED AT 14:59:57 ON 30 JAN 2008

L58 SCREEN 2043 OR 2049 OR 2050  
L59 SCREEN 2003 AND 1839 AND 1993  
L60 10 SEA SSS SAM (L50 NOT ((L40 OR L41 OR L46 OR L47))) AND L59 AND  
L52 NOT L58  
D STAT QUE L54  
L61 SCREEN 1947  
L62 10 SEA SSS SAM (L50 NOT ((L40 OR L41 OR L46 OR L47))) AND L42 AND  
L52 AND L61 NOT L53  
L63 SCREEN 1948  
L64 SCREEN 1949  
L65 SCREEN 1950  
L66 SCREEN 1951  
L67 8 SEA SSS SAM (L50 NOT ((L40 OR L41 OR L46 OR L47))) AND L42 AND  
L52 AND L63 NOT L53  
L68 13 SEA SSS SAM (L50 NOT ((L40 OR L41 OR L46 OR L47))) AND L42 AND  
L52 AND L64 NOT L53  
L69 4 SEA SSS SAM (L50 NOT ((L40 OR L41 OR L46 OR L47))) AND L42 AND  
L52 AND L65 NOT L53  
D QUE NOS L69  
L70 11 SEA SSS SAM (L50 NOT ((L40 OR L41 OR L46 OR L47))) AND L42 AND  
L52 AND L65  
L71 31 SEA SSS SAM (L50 NOT ((L40 OR L41 OR L46 OR L47))) AND L42 AND  
L52 NOT L65  
L72 5 SEA SSS SAM (L50 NOT ((L40 OR L41 OR L46 OR L47))) AND L42 AND  
L52 AND L66  
L73 SCREEN 1952  
L74 SCREEN 1953  
L75 SCREEN 1954  
L76 4 SEA SSS SAM (L50 NOT ((L40 OR L41 OR L46 OR L47))) AND L42 AND  
L52 AND L73  
L77 22 SEA SSS SAM (L50 NOT ((L40 OR L41 OR L46 OR L47))) AND L42 AND  
L52 NOT L73  
L78 50 SEA SSS SAM (L50) AND L42 AND L52 AND L73  
L79 50 SEA SSS SAM (L50) AND L42 AND L52 NOT L73  
L80 978427 SEA SSS FUL (L50) AND L42 AND L52 AND L73 EXTEND  
L81 57965 SEA SSS FUL (L50) AND L42 AND L52 AND L73  
SAVE TEMP L81 BET286FUL1/A  
L82 50 SEA SSS SAM (L50) AND L42 AND L52 NOT L73  
L83 626591 SEA SSS FUL (L50) AND L42 AND L52 NOT L73 EXTEND  
L84 53736 SEA SSS FUL (L50) AND L42 AND L52 NOT L73  
SAVE TEMP L84 BET286FUL2/A  
L85 111701 SEA ABB=ON (L81 OR L84)  
L86 50 SEA SUB=L85 SSS SAM (L40 OR L41 OR L46 OR L47)  
L87 STR L40  
L88 STR L41  
L89 STR L46  
L90 STR L47  
L91 50 SEA SUB=L85 SSS SAM (L50 NOT (L87 OR L88 OR L89 OR L90))  
L92 111701 SEA SUB=L85 SSS FUL (L50 NOT (L87 OR L88 OR L89 OR L90))  
EXTEND



L138 56795 SEA ABB=ON SCREENING/CW  
 L139 4 SEA ABB=ON L130 AND L138  
 D SCAN TI HITIND  
 L140 131348 SEA ABB=ON ASSAY?/OBI  
 L141 2 SEA ABB=ON L130 AND L140  
 L142 269019 SEA ABB=ON FLUORESCEN?/OBI  
 L143 24 SEA ABB=ON L130 AND L142  
 L144 687360 SEA ABB=ON ?ASSAY?/BI  
 L145 24 SEA ABB=ON L130 AND L142 AND L143  
 D QUE  
 L146 9 SEA ABB=ON L130 AND L142 AND L144  
 L147 3612 SEA ABB=ON (PAIN(3A)RECEPTOR#)/BI  
 L148 1 SEA ABB=ON L147 AND L130  
 E EC50/BI  
 L149 19827 SEA ABB=ON EC50/BI  
 E KI/BI  
 L150 90112 SEA ABB=ON KI/BI  
 L151 18813 SEA ABB=ON MICROMOLE#/BI OR MICROMOLAR/BI  
 L152 31 SEA ABB=ON L130 AND (L149 OR L150 OR L151)  
 L153 18 SEA ABB=ON L130 AND (L149 OR L150 OR L151) AND L122  
 D KWIC 1-3  
 L154 5 SEA ABB=ON L130 AND L149  
 L155 25 SEA ABB=ON L130 AND L150  
 L156 1 SEA ABB=ON L130 AND L151  
 L157 6 SEA ABB=ON L130 AND (L149 OR L151)  
 L158 13 SEA ABB=ON L130 AND L150 AND L122  
 L159 2240220 SEA ABB=ON (CONCENTRATION# OR DOSAGE#)/BI  
 L160 4 SEA ABB=ON L159 AND L130 AND L122  
 L161 20 SEA ABB=ON L32 AND (PY<2001 OR AY<2001 OR PRY<2001)  
 L162 10 SEA ABB=ON L161 AND (L12 OR L13 OR L14 OR L15 OR L16 OR L17  
 OR L18 OR L19 OR L20 OR L21 OR L22 OR L23 OR L24 OR L25 OR L26  
 OR L27 OR L28 OR L29 OR L30 OR L31 OR L33 OR L34)

FILE 'STNGUIDE' ENTERED AT 15:37:29 ON 30 JAN 2008

FILE 'HCAPLUS' ENTERED AT 15:37:52 ON 30 JAN 2008

D QUE NOS L96  
 D IBIB ABS HITSTR L96 1-2

FILE 'REGISTRY' ENTERED AT 15:38:27 ON 30 JAN 2008

D STAT QUE L93

FILE 'HCAPLUS' ENTERED AT 15:38:58 ON 30 JAN 2008

D QUE NOS L98  
 D QUE NOS L134  
 D QUE NOS L132  
 D QUE NOS L137

L163 39 SEA ABB=ON (L98 OR L134 OR L132 OR L137) NOT L96  
 D IBIB ABS HITIND HITSTR L163 1-39  
 D QUE NOS L139

L164 3 SEA ABB=ON L139 NOT (L96 OR L163)  
 D IBIB ABS HITIND HITSTR L164 1-3  
 D QUE NOS L141  
 D QUE NOS L146  
 D QUE NOS L148

L165 9 SEA ABB=ON (L141 OR L146 OR L148) NOT (L163 OR L96 OR L164)  
 D IBIB ABS HITIND HITSTR L165 1-9  
 D QUE NOS L160  
 D QUE NOS L151  
 D QUE NOS L158

TITLE: Preparation of diarylpiperazines as capsaicin receptor ligands  
 INVENTOR(S): Bakthavatchalam, Rajagopal  
 PATENT ASSIGNEE(S): Neurogen Corporation, USA; Hutchison, Alan; Desimone, Robert W.; Hodgetts, Keven J.; Krause, James E.; White, Geoffrey G.  
 SOURCE: PCT Int. Appl., 209 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002008221	A2	20020131	WO 2001-US22930	20010720
WO 2002008221	A3	20020711		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2415606	A1	20020131	CA 2001-2415606	20010720
US 2002132853	A1	20020919	US 2001-910442	20010720
US 6723730	B2	20040420		
EP 1301484	A2	20030416	EP 2001-959075	20010720
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001012631	A	20030923	BR 2001-12631	20010720
JP 2004525071	T	20040819	JP 2002-514127	20010720
NZ 523526	A	20041029	NZ 2001-523526	20010720
AU 2001280667	B2	20070802	AU 2001-280667	20010720
MX 2003PA00458	A	20040602	MX 2003-PA458	20030116
US 2004176443	A1	20040909	US 2004-799286	20040312 <--
PRIORITY APPLN. INFO.:				
			US 2000-219529P	P 20000720
			US 2000-230726P	P 20000907
			US 2001-280223P	P 20010330
			US 2001-910442	A1 20010720
			WO 2001-US22930	W 20010720

OTHER SOURCE(S): MARPAT 136:134792

AB Disclosed are diaryl piperazines and related compds. represented by general formula Ar1-A-C(:Z)-NR1-CR3R4-CR3R4-N(R2)Ar2 [I; A = absent, O, S, NRA, CRBRB', NRACRBRB', CRBRB'NRA, -CRA:CRB-, C3H4 (wherein RA, RB, RB' = H, alkyl); Z = O, S; R1, R2 = H, alkyl; R3, R4 = H, halo, HO, NH2, cyano, NO2, CO2H, CHO, each optionally substituted alkyl, alkenyl, alkynyl, alkoxy, mono or dialkylamino, alkylthio, alkyl ketone, alkyl ester, alkylsulfinyl, alkylsulfonyl, mono- or dialkylcarboxamide, -S(O)nNH(alkyl), -S(O)nN(alkyl)(alkyl), -NHCO(alkyl), NHCO(alkyl)(alkyl), -NHS(O)(alkyl), -NS(O)n(alkyl)(alkyl), substituted saturated or partially unsatd. heterocycloalkyl of from 5 to 8 atoms containing 1, 2, or 3 heteroatoms selected from N, O, and S, aryl having from 1 to 3 rings, or heteroaryl; or any two R3 and R4 not attached to the same carbon may be joined to form an each optionally substituted aryl ring, a saturated or partially unsatd. carbocyclic ring of from 5 to 8 members, or a saturated, partially unsatd., or aromatic heterocyclic ring of from 5 to 8 members containing 1, 2, or 3 heteroatoms selected from N, O, and S; Ar1, Ar2 = optionally substituted

SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,  
YU, ZA, ZW  
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,  
CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2379640	A1	20010405	CA 2000-2379640	20000929
CA 2379640	C	20061128		
EP 1224187	A2	20020724	EP 2000-967133	20000929
EP 1224187	B1	20060222		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
HU 2002002636	A2	20021228	HU 2002-2636	20000929
HU 2002002636	A3	20040628		
US 6506762	B1	20030114	US 2000-676941	20000929
JP 2003510327	T	20030318	JP 2001-526541	20000929
NZ 517575	A	20040430	NZ 2000-517575	20000929
AT 318267	T	20060315	AT 2000-967133	20000929
ES 2258476	T3	20060901	ES 2000-967133	20000929
BG 106508	A	20030228	BG 2002-106508	20020311
NO 2002001358	A	20020527	NO 2002-1358	20020319
ZA 2002002518	A	20030630	ZA 2002-2518	20020328
US 2003158197	A1	20030821	US 2002-291446	20021108
US 6696445	B2	20040224		
US 2004229870	A1	20041118	US 2003-705446	20031110
US 7074929	B2	20060711		
JP 2008007515	A	20080117	JP 2007-215782	20070822
PRIORITY APPLN. INFO.:			US 1999-156870P	P 19990930
			JP 2001-526541	A3 20000929
			US 2000-676941	A3 20000929
			WO 2000-US26886	W 20000929
			US 2002-291446	A3 20021108
OTHER SOURCE(S):	MARPAT 134:280854			
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The title compds. [I-III, etc.; X = N, CR14; W = S, O, NR15; Y = N, CR3; E, F, G = CR3, N; R1 = H, alkyl, etc.; R2 = H, alkyl, cycloalkyl, etc.; A = (un)substituted (CH<sub>2</sub>)<sub>m</sub> (wherein m = 1-3); A and B form a (un)substituted carbocycle; A and R2, or B and R2 form (un)substituted aminocarbocycle, aminoheterocycle; B = (un)substituted (CH<sub>2</sub>)<sub>n</sub> (n = 1-3); R3, R16 = H, alkyl, etc.; R4 = (un)substituted aryl, heteroaryl; R5 = (cycloalkyl)alkyl, alkenyl, etc.; R6 = H, alkyl, etc.] which are potent antagonists at the NPY1 receptor, and are useful in treating physiol. disorders associated with an excess of neuropeptide Y, including eating disorders, such as, for example, obesity and bulimia, and certain cardiovascular diseases, for example, hypertension, were prepared. E.g., a multi-step synthesis of IV was described. The compds. I showed K<sub>i</sub> of 0.1 nM - 10 μM against NPY1 receptor binding.

IT 332140-78-0P 332140-80-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of certain alkylene diamine-substituted heterocycles as NPY1 receptor inhibitors)

RN 332140-78-0 HCAPLUS

CN Benzeneacetamide, 4-ethoxy-3-methoxy-N-[2-[[2-methyl-10-(2,4,6-trimethylphenyl)pyrido[2,3-b]indolizin-4-yl]amino]ethyl]- (CA INDEX NAME)

## STRUCTURE + PAIN

=> fil reg; d stat que 193

FILE 'REGISTRY' ENTERED AT 15:38:27 ON 30 JAN 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 JAN 2008 HIGHEST RN 1001040-86-3

DICTIONARY FILE UPDATES: 29 JAN 2008 HIGHEST RN 1001040-86-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

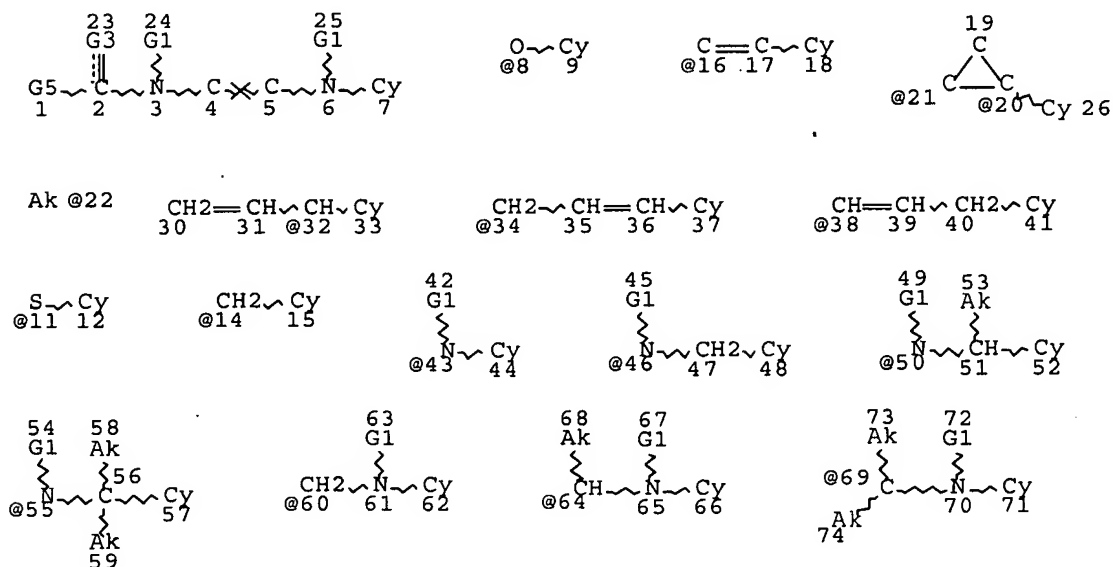
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

L42 SCR 1839 AND 1993

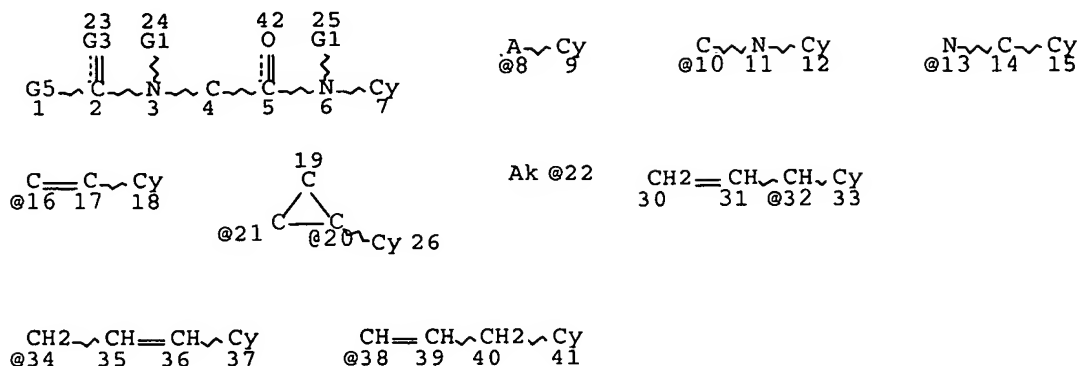
L50 STR



DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 39

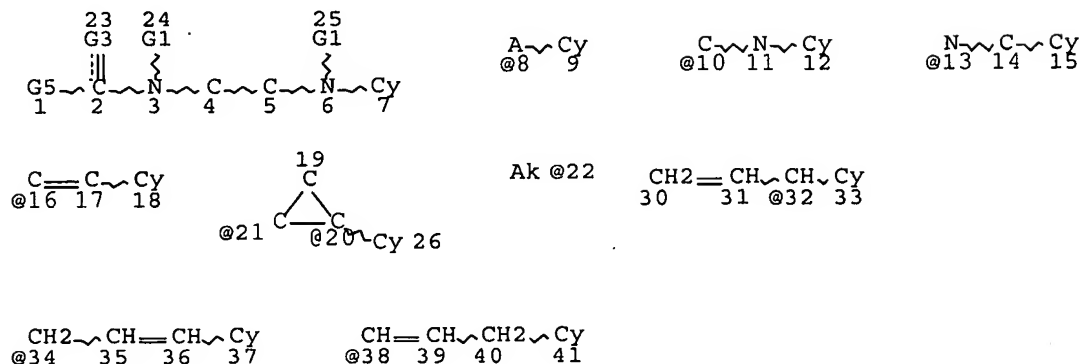
STEREO ATTRIBUTES: NONE  
 L88 STR



VAR G1=H/22  
 VAR G3=O/S  
 VAR G5=CY/8/10/13/16/21/20/32/34/38  
 NODE ATTRIBUTES:  
 CONNECT IS E1 RC AT 22  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 39

STEREO ATTRIBUTES: NONE  
 L89 STR



VAR G1=H/22  
 VAR G3=O/S  
 VAR G5=CY/8/10/13/16/21/20/32/34/38  
 NODE ATTRIBUTES:  
 NSPEC IS RC AT 4

26, 1996), unless otherwise indicated in the original publications.  
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FILE COVERS 1907 - 30 Jan 2008 VOL 148 ISS 5  
 FILE LAST UPDATED: 29 Jan 2008 (20080129/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate  
 substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

L32	416	SEA FILE=HCAPLUS ABB=ON CAPSAICIN RECEPTORS/CT(L) (ANTAG?/OBI OR INHIB?/OBI OR BLOCK?/OBI)
L42		SCR 1839 AND 1993
L50		STR
L52		SCR 392 OR 391
L73		SCR 1952
L81	57965	SEA FILE=REGISTRY SSS FUL (L50) AND L42 AND L52 AND L73
L84	53736	SEA FILE=REGISTRY SSS FUL (L50) AND L42 AND L52 NOT L73
L85	111701	SEA FILE=REGISTRY ABB=ON (L81 OR L84)
L87		STR
L88		STR
L89		STR
L90		STR
L93	8317	SEA FILE=REGISTRY SUB=L85 SSS FUL (L50 NOT (L87 OR L88 OR L89 OR L90))
L94	1407	SEA FILE=HCAPLUS ABB=ON L93
L98	9	SEA FILE=HCAPLUS ABB=ON L32 AND L94
L13	1523	SEA FILE=HCAPLUS ABB=ON NEURITIS/OBI
L14	1695	SEA FILE=HCAPLUS ABB=ON NEURALGI?/OBI
L15	146	SEA FILE=HCAPLUS ABB=ON CAUSALGI?/OBI
L16	355	SEA FILE=HCAPLUS ABB=ON POLYNEURITIS/OBI
L17	32	SEA FILE=HCAPLUS ABB=ON NEURONITIS/OBI
L19	198	SEA FILE=HCAPLUS ABB=ON TOOTHACHE/OBI OR TOOTH/OBI(L)ACHE/OBI
L20	1574	SEA FILE=HCAPLUS ABB=ON BITE#/OBI OR STING#/OBI
L21	214	SEA FILE=HCAPLUS ABB=ON SYMPATHETIC/OBI(L)DYSTROPH?/OBI
L23	1155	SEA FILE=HCAPLUS ABB=ON FIBROMYALGIA/OBI
L24	2	SEA FILE=HCAPLUS ABB=ON GUILLIAN BARRE/OBI
L25	32	SEA FILE=HCAPLUS ABB=ON PARESTHETICA/OBI(L)MERALGI?/OBI
L26	50	SEA FILE=HCAPLUS ABB=ON BURNING MOUTH/OBI
L28	284	SEA FILE=HCAPLUS ABB=ON CHILDBIRTH/OBI
L29	6567	SEA FILE=HCAPLUS ABB=ON MENSTRUUA?/OBI
L30	9	SEA FILE=HCAPLUS ABB=ON LABOR/OBI(L)OBSTETRIC/OBI
L31	1419	SEA FILE=HCAPLUS ABB=ON GUILLAIN BARRE/OBI
L32	416	SEA FILE=HCAPLUS ABB=ON CAPSAICIN RECEPTORS/CT(L) (ANTAG?/OBI OR INHIB?/OBI OR BLOCK?/OBI)
L33	12049	SEA FILE=HCAPLUS ABB=ON PARTURITION/CT
L42		SCR 1839 AND 1993
L50		STR
L52		SCR 392 OR 391

L22 39283 SEA FILE=HCAPLUS ABB=ON ARTHRITIS/OBI  
 L23 1155 SEA FILE=HCAPLUS ABB=ON FIBROMYALGIA/OBI  
 L24 2 SEA FILE=HCAPLUS ABB=ON GUILLIAN BARRE/OBI  
 L25 32 SEA FILE=HCAPLUS ABB=ON PARESTHETICA/OBI (L) MERALGI?/OBI  
 L26 50 SEA FILE=HCAPLUS ABB=ON BURNING MOUTH/OBI  
 L27 7354 SEA FILE=HCAPLUS ABB=ON HEADACHE/OBI OR HEAD/OBI (L) ACHE/OBI  
 L28 284 SEA FILE=HCAPLUS ABB=ON CHILDBIRTH/OBI  
 L29 6567 SEA FILE=HCAPLUS ABB=ON MENSTRUA?/OBI  
 L30 9 SEA FILE=HCAPLUS ABB=ON LABOR/OBI (L) OBSTETRIC/OBI  
 L31 1419 SEA FILE=HCAPLUS ABB=ON GUILLAIN BARRE/OBI  
 L33 12049 SEA FILE=HCAPLUS ABB=ON PARTURITION/CT  
 L34 58509 SEA FILE=HCAPLUS ABB=ON ANALGES?/OBI  
 L42 SCR 1839 AND 1993  
 L50 STR  
 L52 SCR 392 OR 391  
 L73 SCR 1952  
 L81 57965 SEA FILE=REGISTRY SSS FUL (L50) AND L42 AND L52 AND L73  
 L84 53736 SEA FILE=REGISTRY SSS FUL (L50) AND L42 AND L52 NOT L73  
 L85 111701 SEA FILE=REGISTRY ABB=ON (L81 OR L84)  
 L87 STR  
 L88 STR  
 L89 STR  
 L90 STR  
 L93 8317 SEA FILE=REGISTRY SUB=L85 SSS FUL (L50 NOT (L87 OR L88 OR L89  
 OR L90))  
 L94 1407 SEA FILE=HCAPLUS ABB=ON L93  
 L130 912 SEA FILE=HCAPLUS ABB=ON L94 AND (PY<2001 OR AY<2001 OR  
 PRY<2001)  
 L137 2 SEA FILE=HCAPLUS ABB=ON L94 (L) (L12 OR L13 OR L14 OR L15 OR  
 L16 OR L17 OR L19 OR L20 OR L21 OR L22 OR L23 OR L24 OR L25 OR  
 L26 OR L27 OR L28 OR L29 OR L30 OR L31 OR L33 OR L34) AND L130

=> s 198,1134,1132,1137 not 196

L163 39 (L98 OR L134 OR L132 OR L137) NOT L96

=> d ibib abs hitind hitstr 1163 1-39

L163 ANSWER 1 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:1122305 HCAPLUS Full-text

DOCUMENT NUMBER: 147:533963

TITLE: [3H]A-778317 [1-((R)-5-tert-Butyl-indan-1-yl)-3-  
 isoquinolin-5-yl-urea]: a novel, stereoselective,  
 high-affinity antagonist is a useful radioligand for  
 the human transient receptor potential vanilloid-1  
 (TRPV1) receptor

AUTHOR(S): Bianchi, Bruce R.; El Kouhen, Rachid; Neelands, Torben  
 R.; Lee, Chih-Hung; Gomtsyan, Arthur; Raja, Shirish  
 N.; Vaidyanathan, Sriajan N.; Surber, Bruce; McDonald,  
 Heath A.; Surowy, Carol S.; Faltynek, Connie R.;  
 Moreland, Robert B.; Jarvis, Michael F.; Puttfarcken,  
 Pamela S.

CORPORATE SOURCE: Department of Neuroscience Research, Global  
 Pharmaceutical Research and Development, Abbott  
 Laboratories, Abbott Park, IL, USA

SOURCE: Journal of Pharmacology and Experimental Therapeutics  
 (2007), 323(1), 285-293

CODEN: JPETAB; ISSN: 0022-3565

PUBLISHER: American Society for Pharmacology and Experimental  
 Therapeutics

DOCUMENT NUMBER: 147:226990  
 TITLE: Characterization of SB-705498, a potent and selective vanilloid receptor-1 (VR1/TRPV1) antagonist that inhibits the capsaicin-, acid-, and heat-mediated activation of the receptor  
 AUTHOR(S): Gunthorpe, Martin J.; Hannan, Sara Luis; Smart, Darren; Jerman, Jeffrey C.; Arpino, Sandra; Smith, Graham D.; Brough, Stephen; Wright, Jim; Egerton, Julie; Lappin, Sarah C.; Holland, Vicky A.; Winborn, Kim; Thompson, Mervyn; Rami, Harshad K.; Randall, Andrew; Davis, John B.  
 CORPORATE SOURCE: Neurology and Gastrointestinal Centre of Excellence for Drug Discovery, GlaxoSmithKline, Harlow, Essex, UK  
 SOURCE: Journal of Pharmacology and Experimental Therapeutics (2007), 321(3), 1183-1192  
 CODEN: JPETAB; ISSN: 0022-3565  
 PUBLISHER: American Society for Pharmacology and Experimental Therapeutics  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Vanilloid receptor-1 (TRPV1) is a nonselective cation channel, predominantly expressed by sensory neurons, which plays a key role in the detection of noxious painful stimuli such as capsaicin, acid, and heat. TRPV1 antagonists may represent novel therapeutic agents for the treatment of a range of conditions including chronic pain, migraine, and gastrointestinal disorders. Here we describe the in vitro pharmacol. of N-(2-bromophenyl)-N'-[(R)-1-(5-trifluoromethyl-2-pyridyl)pyrrolidin-3-yl]urea (SB-705498), a novel TRPV1 antagonist identified by lead optimization of N-(2-bromophenyl)-N'-{2-[ethyl(3-methylphenyl)amino]ethyl}urea (SB-452533), which has now entered clin. trials. Using a Ca<sup>2+</sup>-based fluorometric imaging plate reader (FLIPR) assay, SB-705498 was shown to be a potent competitive antagonist of the capsaicin-mediated activation of the human TRPV1 receptor (pK<sub>i</sub> = 7.6) with activity at rat (pK<sub>i</sub> = 7.5) and guinea pig (pK<sub>i</sub> = 7.3) orthologs. Whole-cell patch-clamp electrophysiol. was used to confirm and extend these findings, demonstrating that SB-705498 can potentially inhibit the multiple modes of receptor activation that may be relevant to the pathophysiol. role of TRPV1 in vivo: SB-705498 caused rapid and reversible inhibition of the capsaicin (IC<sub>50</sub> = 3 nM)-, acid (pH 5.3)-, or heat (50°; IC<sub>50</sub> = 6 nM)-mediated activation of human TRPV1 (at -70 mV). Interestingly, SB-705498 also showed a degree of voltage dependence, suggesting an effective enhancement of antagonist action at neg. potentials such as those that might be encountered in neurons in vivo. The selectivity of SB-705498 was defined by broad receptor profiling and other cellular assays in which it showed little or no activity vs. a wide range of ion channels, receptors, and enzymes. SB-705498 therefore represents a potent and selective multimodal TRPV1 antagonist, a pharmacol. profile that has contributed to its definition as a suitable drug candidate for clin. development.

CC 1-11 (Pharmacology)

IT Capsaicin receptors

RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 (type VR1; characterization of SB-705498, a potent and selective vanilloid receptor-1 (VR1/TRPV1) antagonist that inhibits the capsaicin-, acid-, and heat-mediated activation of receptor)

IT 459429-39-1D, SB-452533, derivative 501951-42-4, SB 705498

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(characterization of SB-705498, a potent and selective vanilloid receptor-1 (VR1/TRPV1) antagonist that inhibits the capsaicin-, acid-, and heat-mediated activation of receptor)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The invention relates to benzimidazole compds. of formula I, which express dual nitric oxide synthase (NOS) inhibitory activity and agonist activity at the  $\mu$ -opioid receptor. In compds. I, R1 is (un)substituted C1-6 alkyl, (un)substituted C1-4 alkyl-aryl, or (un)substituted C1-4 alkyl-heterocyclyl; R2 is selected from H, halo, (un)substituted C1-6 alkyl, (un)substituted C6-10 aryl, (un)substituted C1-4 alkyl-aryl, (un)substituted C2-9 bridged heterocyclyl, (un)substituted C1-4 alkyl-bridged heterocyclyl, (un)substituted C2-9 heterocyclyl, and (un)substituted C1-4 alkyl-heterocyclyl; R3 and R4 are independently selected from H, F, C1-6 alkyl, and C1-6 alkoxy; R5 is H, R7C(=NH)NH(CH2)p, R7NHC(=NH)NH(CH2)p, or R7NHC(=S)NH(CH2)p, where p is 0-2 and R7 is (un)substituted C1-6 alkyl, (un)substituted C6-10 aryl, (un)substituted C1-4 alkyl-aryl, (un)substituted C2-9 heterocyclyl, etc.; and R6 is H, R8C(=NH)NH(CH2)q, R8NHC(=NH)NH(CH2)q, or R8NHC(=S)NH(CH2)q, where q is 0-2 and R8 is nitro, (un)substituted C1-6 alkyl, (un)substituted C6-10 aryl, (un)substituted C1-4 alkyl-aryl, (un)substituted aroyl, etc.; wherein one, but not both, of R5 and R6 are H; including pharmaceutically acceptable salts or prodrugs thereof. The invention also relates to the preparation of I, pharmaceutical compns. comprising a compound I and a pharmaceutically acceptable excipient, as well to the use of the compns. for the treatment or prevention of chronic pain, acute pain, migraine, and neuropathic pain. Substitution of chloro-2,4-dinitrobenzene with N,N-diethylethylenediamine followed by reduction and amidation with 4-ethoxyphenylacetic acid gave amide II, which underwent intramol. heterocyclization, hydrogenation, and coupling with Me thiophene-2-carboximidothioate hydriodide to give benzimidazole III. The compds. of the invention have dual activity as NOS inhibitors and  $\mu$ -opioid agonists as exemplified by compound III, which expresses IC50 values of 0.44  $\mu$ M and 4.7  $\mu$ M towards human neuronal NOS and human endothelial NOS, resp., and IC50 value of 13 nM for binding and EC50 of 0.34  $\mu$ M for function of  $\mu$ -opioid receptors.

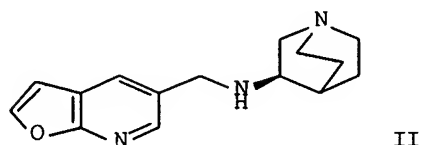
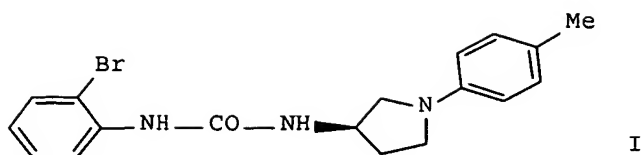
IC ICM C07D

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1, 63

IT Capsaicin receptors

RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(type VR1; preparation of benzimidazole compds. as dual nitric oxide synthase inhibitors and  $\mu$ -opioid agonists)

IT 911-65-9P, N-[2-[2-(4-Ethoxybenzyl)-5-nitrobenzimidazol-1-yl]ethyl]diethylamine 4119-48-6P, N'-(2,4-Dinitrophenyl)-N,N-dimethylethane-1,2-diamine 5099-39-8P, 1-[(2-Diethylaminoethyl)amino]-4-nitrobenzene-2-amine 55154-71-7P, N-[2-(2-Diethylaminoethylamino)-5-nitrophenyl]-2-(4-ethoxyphenyl)acetamide 56223-91-7P, N'-(2,4-Dinitrophenyl)-N,N-diethylethane-1,2-diamine 56756-68-4P, 1-[(2-Dimethylaminoethyl)amino]-4-nitrobenzene-2-amine 102517-00-0P, 2-(4-Ethoxybenzyl)-5-nitro-1H-benzimidazole 114160-61-1P, N-[2-[2-(4-Ethoxybenzyl)-6-nitrobenzimidazol-1-yl]ethyl]diethylamine 714190-52-0P, [2-[2-(4-Ethoxybenzyl)-5-nitrobenzimidazol-1-yl]ethyl]dimethylamine 925216-50-8P, N-[2-(2-Dimethylaminoethylamino)-5-nitrophenyl]-2-(4-ethoxyphenyl)acetamide 925216-67-7P, [1-(2-Diethylaminoethyl)-2-(4-ethoxybenzyl)-1H-benzimidazol-5-yl]thiourea 925216-69-9P, (2,4-Dinitrophenyl)[2-(1-methylpyrrolidin-2-yl)ethyl]amine 925216-70-2P, 1-[[2-(1-Methylpyrrolidin-2-yl)ethyl]amino]-4-nitrobenzene-2-amine 925216-71-3P, 2-(4-Ethoxyphenyl)-N-[2-[[2-(1-methylpyrrolidin-2-yl)ethyl]amino]-5-nitrophenyl]acetamide 925216-74-6P,



AB Small mol. antagonists of the vanilloid receptor TRPV1 (also known as VR1) are disclosed. Pyrrolidinyl ureas such as (I) and (II) (SB-705498) emerged as lead compds. following optimization of the previously described urea SB-452533. Pharmacol. studies using electrophysiol. and FLIPR-Ca<sup>2+</sup>-based assays showed that compds. such as I and II were potent antagonists vs. the multiple chemical and phys. modes of TRPV1 activation (namely capsaicin, acid and noxious heat). Furthermore, II possessed suitable lead compound properties to enable progression of this compound into in vivo studies and subsequently clin. development.

CC 1-3 (Pharmacology)  
Section cross-reference(s): 27

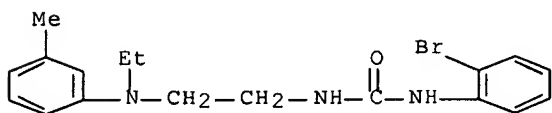
IT Capsaicin receptors  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(type VR1; SB-705498, a potent, selective and orally bioavailable TRPV1 antagonist suitable for clin. development)

IT 459429-39-1, SB-452533  
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(SB-705498, a potent, selective and orally bioavailable TRPV1 antagonist suitable for clin. development)

IT 459429-39-1, SB-452533  
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(SB-705498, a potent, selective and orally bioavailable TRPV1 antagonist suitable for clin. development)

RN 459429-39-1 HCAPLUS

CN Urea, N-(2-bromophenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]- (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 5 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:1170872 HCAPLUS Full-text  
 DOCUMENT NUMBER: 143:440424  
 TITLE: Preparation of benzoxazinylurea analogs as VR1

NR1R2 = 5-12 membered (un)substituted (un)saturated cyclic ring; R3 = H, alk(en/yn)yl; each R4 = independently H, nO2, OH, SH, CN, etc.; m = 1-3; X = O, CH2, S, NH, N-alkyl] which are useful as active ingredients of pharmaceutical preps. Compds. I have an excellent activity as VR1 antagonists. E.g., a 4-step synthesis, starting from 2-amino-4-nitrophenol, was given for urea II. Capsaicin-induced Ca<sup>2+</sup> influx in the human VR1-transfected CHO cell line in the presence of II was 24 nM. I are useful for the prophylaxis and treatment of diseases associated with VR1 activity, in particular for the treatment of urol. disorder or disease, such as detrusor overactivity (overactive bladder), urinary incontinence, neurogenic detrusor overactivity (detrusor hyperflexia), idiopathic detrusor overactivity (detrusor instability), benign prostatic hyperplasia, and lower urinary tract symptoms; chronic pain, neuropathic pain, postoperative pain, rheumatoid arthritic pain, neuralgia, neuropathies, algesia, nerve injury, ischemia, neurodegeneration, stroke; and respiratory diseases and inflammatory disorders such as asthma, chronic obstructive pulmonary (or airways) disease (COPD), common cold, cough, sneeze, bronchitis including acute and chronic bronchitis, bronchiolitis, rhinitis, allergic rhinitis, vasomotor rhinitis, mucositis, sinusitis, allergy, disorders associated with exogenous irritants such as tobacco smoke, smog, high levels of atmospheric SO<sub>2</sub> and noxious gases in the workplace, and airways hyperreactivity, milk product intolerance, Loffler's pneumonia, emphysema, cystic fibrosis, bronchiectasis, pulmonary fibrosis, pneumoconiosis, collagen vascular disease, granulomatous disease, laryngitis, pharyngitis, pneumonia, pleuritis, persistent asthma and chronic asthmatic bronchitis.

IC ICM C07D265-36

ICS C07D215-227; A61K031-538; A61P013-02

CC 28-13 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

IT Capsaicin receptors

RL: BSU (Biological study, unclassified); BIOL (Biological study)

(type VR1; preparation of benzoxazinylurea analogs as vanilloid receptor

VR1

antagonists)

IT 868593-15-1P, N-[2-[Ethyl(3-methylphenyl)amino]ethyl]-N'-(3-oxo-

3,4-dihydro-2H-1,4-benzoxazin-6-yl)urea 868593-16-2P,

1-[2-[Ethyl(3-methylphenyl)amino]ethyl]-3-(2-oxo-1,2,3,4-

tetrahydroquinolin-5-yl)urea

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)

(drug candidate; preparation of benzoxazinylurea analogs as vanilloid receptor VR1 antagonists)

IT 868593-15-1P, N-[2-[Ethyl(3-methylphenyl)amino]ethyl]-N'-(3-oxo-

3,4-dihydro-2H-1,4-benzoxazin-6-yl)urea 868593-16-2P,

1-[2-[Ethyl(3-methylphenyl)amino]ethyl]-3-(2-oxo-1,2,3,4-

tetrahydroquinolin-5-yl)urea

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)

(drug candidate; preparation of benzoxazinylurea analogs as vanilloid receptor VR1 antagonists)

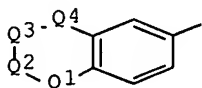
RN 868593-15-1 HCAPLUS

CN Urea, N-(3,4-dihydro-3-oxo-2H-1,4-benzoxazin-6-yl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]- (CA INDEX NAME)

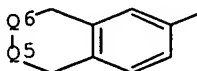
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 EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,  
 SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,  
 SN, TD, TG

CA 2545100	A1	20050519	CA 2004-2545100	20041026
EP 1687262	A1	20060809	EP 2004-790835	20041026
R: DE, ES, FR, GB, IT				
JP 2007511479	T	20070510	JP 2006-538690	20041026
PRIORITY APPLN. INFO.:			EP 2003-25571	A 20031108
			EP 2003-27003	A 20031122
			WO 2004-EP12050	W 20041026
OTHER SOURCE(S):		CASREACT 142:463465; MARPAT 142:463465		
GI				

Q7=



Q8=



AB This invention relates to bicyclic amide, carbamate or urea derivs. of formula A-NHCO-Y-(CH<sub>2</sub>)<sub>m</sub>-X-(CH<sub>2</sub>)<sub>p</sub>-R1 and salts thereof [A = Q7, Q8; wherein Q1, Q4 = direct bond, methylene; Q2 = CHR2, or CO; Q3 = CHR3 or CO (wherein R2, R3 = H, HO, C1-6 alkoxy, C1-6 alkanoyloxy or (un)substituted 1-6 alkyl); with the proviso that Q1 and Q4 can be direct bond t the same time; R2 = R3 ≠ H; when Q = direct nd, then R3 = HO, C1-6 alkoxy, or C1-6 alkanoyloxy; Q5 = CH or R5 (wherein R5 = HO, C1-6 alkoxy, C1-6 alkanoyloxy, or (un)substituted C1-6 alkyl); Q6 = CH or CR6 (wherein R6 = HO, C1-6 alkoxy, C1-6 alkanoyloxy, or (un)substituted C1-6 alkyl); with the proviso that Q5 ≠ Q6 = CH; m = 0-3; p = 0, 1; X = a bond, O, NR4 (wherein R4 = H, C1-6 alkyl), with the proviso that when m = 0, then X = a bond; Y = CH2, O or NH; R1 = each (un)substituted aryl or heteroaryl] which are useful as active ingredients of pharmaceutical prepn's. The bicyclic amide, carbamate or urea derivs. of the resent invention has vanilloid receptor (VR1) antagonistic activity (no data). These compds. can be used for the prophylaxis and treatment of diseases associated with VR1 activity, in particular for the treatment of urol. diseases or disorders such as detrusor overactivity (overactive bladder), urinary incontinence, neurogenic detrusor overactivity (detrusor hyperflexia), idiopathic detrusor overactivity (detrusor instability), benign prostatic hyperplasia, and lower urinary tract symptoms; pain such as chronic pain, neuropathic pain, postoperative pain, rheumatoid arthritic pain, neuralgia, neuropathies, algesia, nerve injury, ischemia, neurodegeneration, and stroke; and inflammatory disorders such as asthma and chronic obstructive pulmonary (or airways) disease (COPD). Thus, a mixture of 70.0 mg 7-amino-1,2,3,4-tetrahydronaphthalen-2-ol and 95.0 mg 4-chloro-3-trifluoromethylphenyl isocyanate in 10 mL DMF was stirred at 50° for 2 h, concentrated under reduced pressure, and purified by silica gel chromatog. to give 49.9 mg N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-(7-hydroxy-5,6,7,8-tetrahydronaphthalen-2-yl)urea.

IC ICM C07C275-28

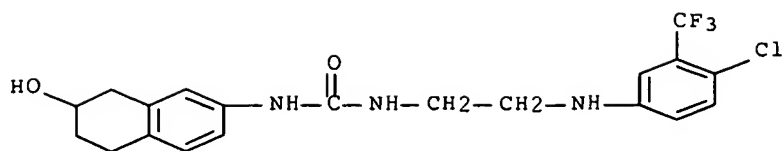
ICS C07C275-32; C07C235-38; A61K031-16; A61K031-17

CC 25-27 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 Section cross-reference(s): 1

IT Capsaicin receptors

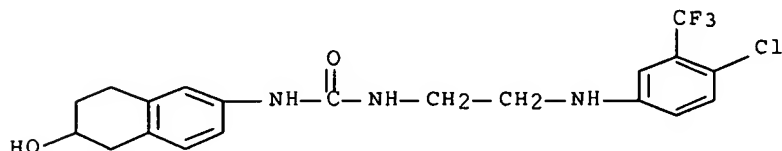
RL: BSU (Biological study, unclassified); BIOL (Biological study)

(type VR1; preparation of bicyclic amides, carbamates or urea derivs. as



RN 851773-91-6 HCAPLUS

CN Urea, N-[2-[[4-chloro-3-(trifluoromethyl)phenyl]amino]ethyl]-N'-(5,6,7,8-tetrahydro-6-hydroxy-2-naphthalenyl)- (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 7 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:696338 HCAPLUS Full-text

DOCUMENT NUMBER: 141:225165

TITLE: Preparation of hydroxytetrahydronaphthalenylurea derivatives as VR1 antagonists for the prophylaxis and treatment of diseases associated with VR1 activity, such as urological diseases, pain and inflammatory diseases

INVENTOR(S): Yura, Takeshi; Mogi, Muneto; Fujishima, Hiroshi; Urbahns, Klaus; Masuda, Tsutomu; Tsukimi, Yasuhiro; Tajimi, Masaomi; Yamamoto, Noriyuki; Yoshida, Nagahiro; Moriwaki, Toshiya

PATENT ASSIGNEE(S): Bayer Healthcare AG, Germany; et al.

SOURCE: PCT Int. Appl., 57 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004072020	A1	20040826	WO 2004-EP1055	20040205
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2515418	A1	20040826	CA 2004-2515418	20040205
EP 1594836	A1	20051116	EP 2004-708355	20040205
EP 1594836	B1	20070919		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,			

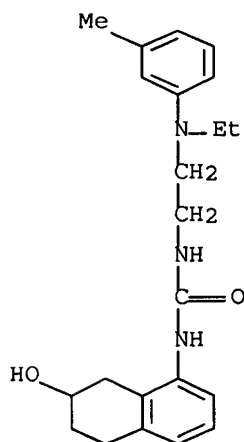
CC 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 Section cross-reference(s): 1, 63

IT Capsaicin receptors  
 RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 (type VR1, antagonists; preparation of  
 hydroxytetrahydronaphthalenylurea derivs. as VR1 antagonists)

IT 745784-14-9P 745784-15-0P 745784-16-1P 745784-17-2P 745784-18-3P  
 745784-19-4P 745784-20-7P 745784-21-8P 745784-22-9P  
 745784-23-0P 745784-24-1P 745784-25-2P  
 745784-26-3P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)  
 (drug candidate; preparation of hydroxytetrahydronaphthalenylurea derivs.  
 as  
 VR1 antagonists)

IT 745784-22-9P 745784-23-0P 745784-24-1P  
 745784-25-2P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)  
 (drug candidate; preparation of hydroxytetrahydronaphthalenylurea derivs.  
 as  
 VR1 antagonists)

RN 745784-22-9 HCAPLUS  
 CN Urea, N-[2-[ethyl(3-methylphenyl)amino]ethyl]-N'-(5,6,7,8-tetrahydro-7-  
 hydroxy-1-naphthalenyl)- (CA INDEX NAME)



RN 745784-23-0 HCAPLUS  
 CN Urea, N-[2-[methyl(3-methylphenyl)amino]ethyl]-N'-(5,6,7,8-tetrahydro-7-  
 hydroxy-1-naphthalenyl)- (CA INDEX NAME)

CORPORATE SOURCE: Neurology and GI CEDD, GlaxoSmithKline, Essex, CM19  
5AW, UK  
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004),  
14(14), 3631-3634  
CODEN: BMCLE8; ISSN: 0960-894X  
PUBLISHER: Elsevier Science B.V.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Small mol. antagonists of the vanilloid receptor 1 (TRPV1, also known as VR1) are disclosed. Ureas such as 5 (SB-452533) were used to explore the structure activity relation with several potent analogs identified. Pharmacol. studies using electrophysiol. and FLIPR Ca<sup>2+</sup> based assays showed compound 5 was an antagonist vs. capsaicin, noxious heat and acid mediated activation of TRPV1. Study of a quaternary salt of 5 supports a mode of action in which compds. from this series cause inhibition via an extracellularly accessible binding site on the TRPV1 receptor.

CC 1-3 (Pharmacology)

IT Capsaicin receptors

RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(type VR1; structure activity of antagonists of TRPV1)

IT 108623-11-6 459429-39-1 459429-44-8  
459429-55-1 459429-56-2 459429-59-5  
459429-60-8 459429-67-5 459429-68-6  
725746-48-5 725746-49-6 725746-50-9  
725746-51-0 725746-52-1 725746-53-2  
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725746-58-7 725746-59-8

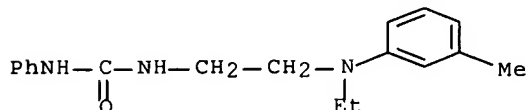
RL: PAC (Pharmacological activity); BIOL (Biological study)  
(structure activity of antagonists of TRPV1)

IT 108623-11-6 459429-39-1 459429-44-8  
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459429-60-8 459429-67-5 459429-68-6  
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725746-56-5 725746-57-6 725746-58-7  
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RL: PAC (Pharmacological activity); BIOL (Biological study)  
(structure activity of antagonists of TRPV1)

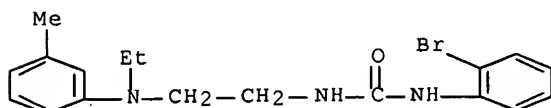
RN 108623-11-6 HCAPLUS

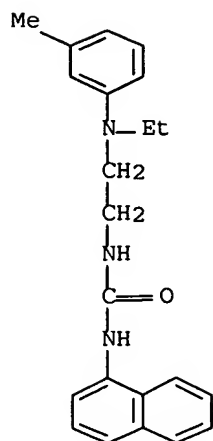
CN Urea, N-[2-[ethyl(3-methylphenyl)amino]ethyl]-N'-phenyl- (CA INDEX NAME)



RN 459429-39-1 HCAPLUS

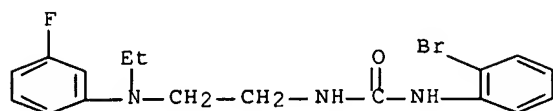
CN Urea, N-(2-bromophenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]- (CA INDEX NAME)





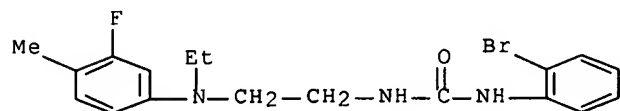
RN 459429-60-8 HCAPLUS

CN Urea, N-(2-bromophenyl)-N'-[2-[ethyl(3-fluorophenyl)amino]ethyl]- (CA INDEX NAME)



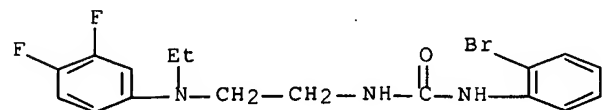
RN 459429-67-5 HCAPLUS

CN Urea, N-(2-bromophenyl)-N'-[2-[ethyl(3-fluoro-4-methylphenyl)amino]ethyl]- (CA INDEX NAME)



RN 459429-68-6 HCAPLUS

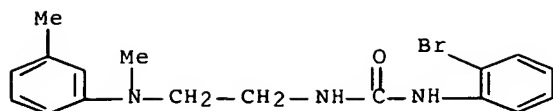
CN Urea, N-(2-bromophenyl)-N'-[2-[(3,4-difluorophenyl)ethylamino]ethyl]- (CA INDEX NAME)



RN 725746-48-5 HCAPLUS

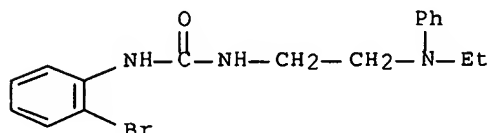
CN Urea, N-[2-[ethyl(3-methylphenyl)amino]ethyl]-N'-(2-methylphenyl)- (CA INDEX NAME)





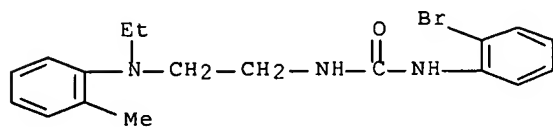
RN 725746-56-5 HCAPLUS

CN Urea, N-(2-bromophenyl)-N'-[2-(2-methylphenylamino)ethyl]- (CA INDEX NAME)



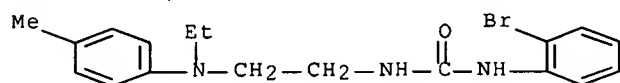
RN 725746-57-6 HCAPLUS

CN Urea, N-(2-bromophenyl)-N'-[2-[ethyl(2-methylphenyl)amino]ethyl]- (CA INDEX NAME)



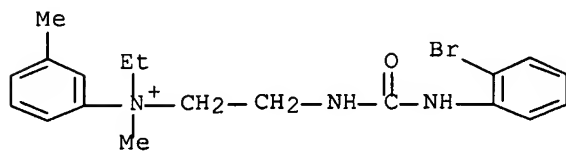
RN 725746-58-7 HCAPLUS

CN Urea, N-(2-bromophenyl)-N'-[2-[ethyl(4-methylphenyl)amino]ethyl]- (CA INDEX NAME)



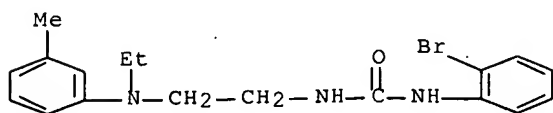
RN 725746-59-8 HCAPLUS

CN Benzenaminium, N-[2-[[[(2-bromophenyl)amino]carbonyl]amino]ethyl]-N-ethyl-N,3-dimethyl-, iodide (9CI) (CA INDEX NAME)



● I<sup>-</sup>

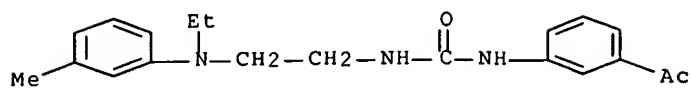
- AB The title compds. [I; P = Ph, naphthyl; R1 = halo, alkyl, CF3, etc.; p = 0-3; n = 2-6; R2 = halo, alkyl, CF3, etc.; q = 0-3; R3 = H, alkyl, arylalkyl] having vanilloid receptor (VR1) antagonist activity, and therefore useful in the treatment of various disorders such as pain, migraine, neuralgia, etc., were prepared Thus, reacting N-ethyl-N-(3-methylphenyl)ethylenediamine with 2-bromophenyl isocyanate in DCM afforded 86% II. All compds. I tested against VR1 had pKb > 6.
- IC ICM C07C275-40  
ICS C07C275-34; C07C275-30; C07C275-32; C07C275-28; C07C323-44; A61K031-17; A61P029-00
- CC 25-21 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
Section cross-reference(s): 1
- IT Capsaicin receptors  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(VR1; preparation of ureas having vanilloid receptor (VR1) antagonist activity)
- IT 459429-39-1P 459429-41-5P 459429-42-6P  
459429-43-7P 459429-44-8P 459429-45-9P  
459429-46-0P 459429-47-1P 459429-48-2P  
459429-49-3P 459429-50-6P 459429-51-7P  
459429-52-8P 459429-53-9P 459429-54-0P  
459429-55-1P 459429-56-2P 459429-57-3P  
459429-58-4P 459429-59-5P 459429-60-8P  
459429-61-9P 459429-62-0P 459429-63-1P  
459429-64-2P 459429-65-3P 459429-66-4P  
459429-67-5P 459429-68-6P 459429-69-7P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of ureas having vanilloid receptor (VR1) antagonist activity)
- IT 459429-39-1P 459429-41-5P 459429-42-6P  
459429-43-7P 459429-44-8P 459429-45-9P  
459429-46-0P 459429-47-1P 459429-48-2P  
459429-49-3P 459429-50-6P 459429-51-7P  
459429-52-8P 459429-53-9P 459429-54-0P  
459429-55-1P 459429-56-2P 459429-57-3P  
459429-58-4P 459429-59-5P 459429-60-8P  
459429-61-9P 459429-62-0P 459429-63-1P  
459429-64-2P 459429-65-3P 459429-66-4P  
459429-67-5P 459429-68-6P 459429-69-7P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of ureas having vanilloid receptor (VR1) antagonist activity)
- RN 459429-39-1 HCAPLUS
- CN Urea, N-(2-bromophenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]- (CA INDEX NAME)



RN 459429-41-5 HCAPLUS

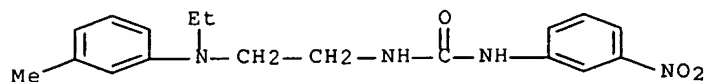
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CN Urea, N-(3-acetylphenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]-(CA INDEX NAME)



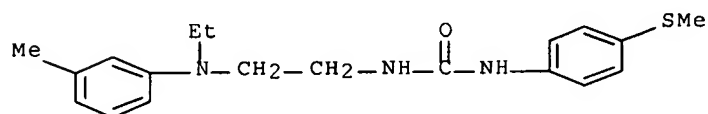
RN 459429-47-1 HCAPLUS

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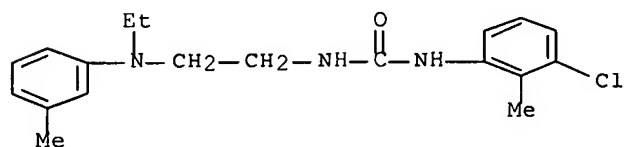
RN 459429-48-2 HCAPLUS

CN Urea, N-[2-[ethyl(3-methylphenyl)amino]ethyl]-N'-[4-(methylthio)phenyl]-(CA INDEX NAME)



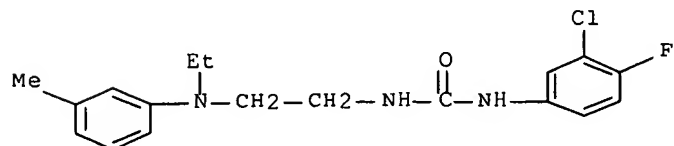
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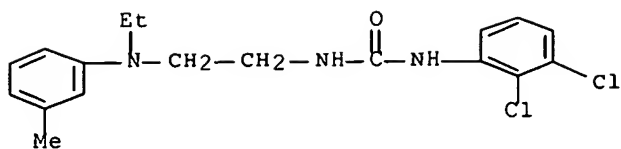
CN Urea, N-(3-chloro-2-methylphenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]-(CA INDEX NAME)



RN 459429-50-6 HCAPLUS

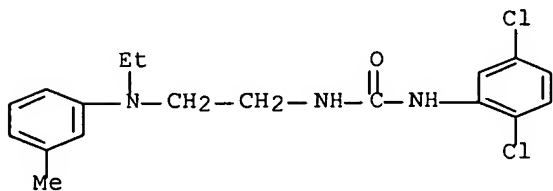
CN Urea, N-(3-chloro-4-fluorophenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]-(CA INDEX NAME)





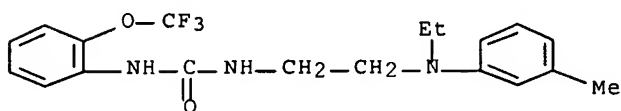
RN 459429-56-2 HCAPLUS

CN Urea, N-(2,5-dichlorophenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]-  
(CA INDEX NAME)



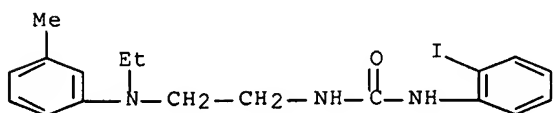
RN 459429-57-3 HCAPLUS

CN Urea, N-[2-[ethyl(3-methylphenyl)amino]ethyl]-N'-[2-(trifluoromethoxy)phenyl]- (CA INDEX NAME)



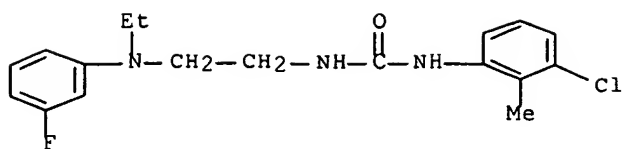
RN 459429-58-4 HCAPLUS

CN Urea, N-[2-[ethyl(3-methylphenyl)amino]ethyl]-N'-(2-iodophenyl)- (CA INDEX NAME)



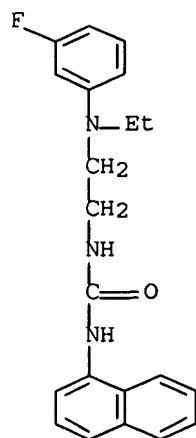
RN 459429-59-5 HCAPLUS

CN Urea, N-[2-[ethyl(3-methylphenyl)amino]ethyl]-N'-1-naphthalenyl- (CA INDEX NAME)



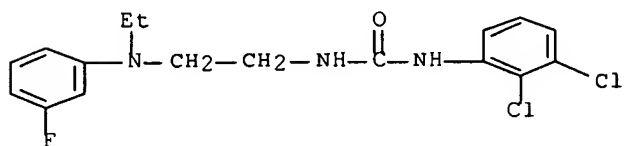
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CN Urea, N-[2-[ethyl(3-fluorophenyl)amino]ethyl]-N'-1-naphthalenyl- (CA INDEX NAME)



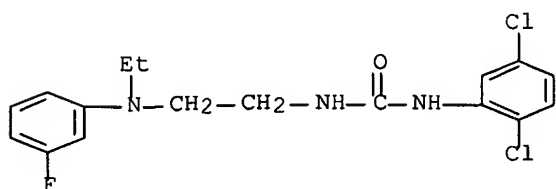
RN 459429-65-3 HCAPLUS

CN Urea, N-(2,3-dichlorophenyl)-N'-[2-[ethyl(3-fluorophenyl)amino]ethyl]- (CA INDEX NAME)



RN 459429-66-4 HCAPLUS

CN Urea, N-(2,5-dichlorophenyl)-N'-[2-[ethyl(3-fluorophenyl)amino]ethyl]- (CA INDEX NAME)



RN 459429-67-5 HCAPLUS

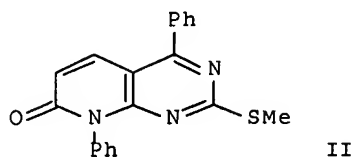
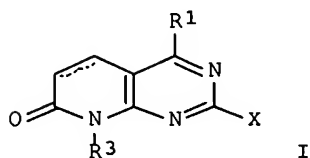
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 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,  
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CA 2426654	A1	20020801	CA 2001-2426654	20011023 <--
AU 2002246855	A1	20020806	AU 2002-246855	20011023 <--
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US 7323472	B2	20080129		
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PRIORITY APPLN. INFO.:

US 2000-242461P	P	20001023 <--
US 2001-310349P	P	20010806
US 2001-326618P	P	20011002
CN 2001-817819	A3	20011023
NZ 2001-524806	A1	20011023
WO 2001-US50493	W	20011023
US 2003-399614	A3	20030418

OTHER SOURCE(S): MARPAT 137:140533  
 GI



AB Title compds. I [wherein X = R2, OR2, SO0-2R2, (CH2)nNR10SO0-2R2, (CH2)nNR10COR2, (CH2)nNR4R14, or (CH2)nN(R2)2; R1 = (un)substituted (hetero)aryl; R2 = H, (un)substituted alkyl, cycloalkyl(alkyl), (hetero)aryl(alkyl), heterocyclyl(alkyl), alkylamino, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, etc.; R3 = (un)substituted alkyl, cycloalkyl(alkyl), (hetero)aryl(alkyl), or heterocyclyl; R4 and R14 =

(synovitis; preparation of pyridopyrimidinones as CSBP/RK/p38 kinase inhibitors by cyclization reactions of (phenylamino)pyrimidinecarbaldehyde derivs.)

IT 444605-70-3P, 8-Cyclopropyl-4-(2-fluorophenyl)-2-methylsulfanyl-8H-pyrido[2,3-d]pyrimidin-7-one 444605-98-5P, 8-sec-Butyl-4-(2-fluorophenyl)-2-methanesulfonyl-8H-pyrido[2,3-d]pyrimidin-7-one 444606-12-6P, 2-(2-Diethylaminoethylamino)-4,8-diphenyl-8H-pyrido[2,3-d]pyrimidin-7-one 444606-13-7P, 2-(2-Diethylaminoethylamino)-8-(2,6-difluorophenyl)-4-(4-fluoro-2-methylphenyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444606-14-8P, 4,8-Bis(2-chlorophenyl)-2-(2-diethylaminoethylamino)-8H-pyrido[2,3-d]pyrimidin-7-one 444606-16-0P, 8-(2-Chlorophenyl)-2-(2-diethylaminoethylamino)-4-(2-fluorophenyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444606-18-2P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-[(2-hydroxy-1-hydroxymethylethyl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444606-19-3P, 4,8-Bis(2-chlorophenyl)-2-[(2-hydroxy-1-hydroxymethylethyl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444606-21-7P, 4-(2-Fluorophenyl)-8-(1-ethylpropyl)-2-[(2-hydroxy-1-hydroxymethylethyl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444606-25-1P, 4-(2-Chlorophenyl)-8-(1-ethylpropyl)-2-[(2-hydroxy-1-hydroxymethylethyl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444606-27-3P, 4-(2-Fluorophenyl)-2-[(2-hydroxy-1-hydroxymethylethyl)amino]-8-isopropyl-8H-pyrido[2,3-d]pyrimidin-7-one 444606-29-5P, 8-Cyclopropyl-4-(4-fluoro-2-methylphenyl)-2-[(2-hydroxy-1-hydroxymethylethyl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444606-31-9P, 8-Cyclopropylmethyl-4-(2-fluorophenyl)-2-[(2-hydroxy-1-hydroxymethylethyl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444606-32-0P, 8-sec-Butyl-4-(4-fluoro-2-methylphenyl)-2-[(2-hydroxy-1-hydroxymethylethyl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444606-33-1P, 4-(4-Fluoro-2-methylphenyl)-8-(2-fluorophenyl)-2-[(2-hydroxy-1-hydroxymethylethyl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444606-35-3P, 4,8-Bis(2-fluorophenyl)-2-[(2-hydroxy-1-hydroxymethylethyl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444606-37-5P, 8-(2,6-Difluorophenyl)-4-(2-fluorophenyl)-2-[(2-hydroxy-1-hydroxymethylethyl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444606-39-7P, 8-Cyclopropylmethyl-4-(4-fluoro-2-methylphenyl)-2-[(2-hydroxy-1-hydroxymethylethyl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444606-40-0P, 4-(4-Fluoro-2-methylphenyl)-2-[(2-hydroxy-1-hydroxymethylethyl)amino]-8-isopropyl-8H-pyrido[2,3-d]pyrimidin-7-one 444606-41-1P, 4,8-Bis(2-chlorophenyl)-2-[(2-dimethylaminoethyl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444606-42-2P, 4,8-Bis(2-chlorophenyl)-2-(piperidin-4-ylamino)-8H-pyrido[2,3-d]pyrimidin-7-one 444606-45-5P, 4,8-Bis(2-chlorophenyl)-2-(1-methylpiperidin-4-ylamino)-8H-pyrido[2,3-d]pyrimidin-7-one 444606-47-7P, 4,8-Bis(2-chlorophenyl)-2-[(2-hydroxy-1-hydroxymethyl-1-methylethyl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444606-49-9P, 4,8-Bis(2-chlorophenyl)-2-(2-hydroxyethylamino)-8H-pyrido[2,3-d]pyrimidin-7-one 444606-51-3P, 2-(2-Aminoethylamino)-4,8-bis(2-chlorophenyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444606-55-7P, [[4,8-Bis(2-chlorophenyl)-7-oxo-7,8-dihydropyrido[2,3-d]pyrimidin-2-yl]amino]acetic acid 444606-56-8P, 4-(2-Chlorophenyl)-2-[(2-diethylaminoethyl)amino]-8-(1-ethylpropyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444606-58-0P, 2-(2-Aminoethylamino)-4-(2-chlorophenyl)-8-(1-ethylpropyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444606-59-1P, 4-(2-Chlorophenyl)-8-(1-ethylpropyl)-2-(2-hydroxyethylamino)-8H-pyrido[2,3-d]pyrimidin-7-one 444606-61-5P, 4-(2-Chlorophenyl)-8-(1-ethylpropyl)-2-[(R)-2-hydroxy-1-methylethyl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444606-62-6P, 4-(2-Chlorophenyl)-8-(1-ethylpropyl)-2-[(1-methylpiperidin-4-yl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444606-63-7P, [[4-(2-Chlorophenyl)-8-(1-ethylpropyl)-7-oxo-7,8-dihydropyrido[2,3-d]pyrimidin-2-yl]amino]acetic acid ethyl ester 444606-65-9P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-(2-hydroxyethylamino)-8H-pyrido[2,3-d]pyrimidin-7-one 444606-67-1P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-[(1-methylpiperidin-4-yl)amino]-8H-pyrido[2,3-

yl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444607-44-7P,  
 2-Hydroxy-4-(4-fluoro-2-methylphenyl)-8-(2-fluorophenyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-45-8P, 2-Cyclohexylamino-4-(4-fluoro-2-methylphenyl)-8-(2-fluorophenyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-46-9P, 2-(Tetrahydropyran-4-ylamino)-4-(4-fluoro-2-methylphenyl)-8-(2-fluorophenyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-47-0P,  
 2-Ethylamino-4-(4-fluoro-2-methylphenyl)-8-(2,6-difluorophenyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-48-1P, 2-Cyclohexylamino-4-(4-fluoro-2-methylphenyl)-8-(2,6-difluorophenyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-49-2P, 2-(Tetrahydropyran-4-ylamino)-4-(4-fluoro-2-methylphenyl)-8-(2,6-difluorophenyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-50-5P,  
 2-(2,2,2-Trifluoroethylamino)-4-(4-fluoro-2-methylphenyl)-8-(2-fluorophenyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-51-6P,  
 trans-2-(4-Hydroxycyclohexylamino)-4-(4-fluoro-2-methylphenyl)-8-(2-fluorophenyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-52-7P,  
 2-[(1-Hydroxymethyl-1-methyl-2-hydroxyethyl)amino]-4-(4-fluoro-2-methylphenyl)-8-(2-fluorophenyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-53-8P, 2-(2,2,2-Trifluoroethylamino)-4-(4-fluoro-2-methylphenyl)-8-(2,6-difluorophenyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-54-9P,  
 trans-2-(4-Hydroxycyclohexylamino)-4-(4-fluoro-2-methylphenyl)-8-(2,6-difluorophenyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-55-0P,  
 2-Ethoxy-4-(4-fluoro-2-methylphenyl)-8-(2-fluorophenyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444607-57-2P, 1-[2-[[8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-7-oxo-7,8-dihydropyrido[2,3-d]pyrimidin-2-yl]amino]ethyl]-3-ethylurea 444607-58-3P, 1-[2-[[8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-7-oxo-7,8-dihydropyrido[2,3-d]pyrimidin-2-yl]amino]ethyl]-3-phenylurea 444607-59-4P,  
 1-[2-[[8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-7-oxo-7,8-dihydropyrido[2,3-d]pyrimidin-2-yl]amino]ethyl]-3-cyclohexylurea 444607-60-7P, 1-[2-[[8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-7-oxo-7,8-dihydropyrido[2,3-d]pyrimidin-2-yl]amino]ethyl]-3-(3-fluorophenyl)urea 444607-61-8P 444607-62-9P 444607-63-0P  
 444607-64-1P 444607-65-2P 444607-66-3P 444607-67-4P 444607-69-6P  
 444607-70-9P 444607-71-0P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-[N-(2,2-dimethyl-2-hydroxyethyl)amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444607-72-1P 444607-73-2P 444607-74-3P  
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 8-Cyclohexyl-4-(4-fluoro-2-methylphenyl)-2-ethoxy-8H-pyrido[2,3-d]pyrimidin-7-one 444607-85-6P 444607-86-7P 444607-87-8P  
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 4-(4-Fluoro-2-methylphenyl)-2-((R)-2-hydroxy-1-methylethylamino)-8-o-tolyl-8H-pyrido[2,3-d]pyrimidin-7-one 444607-97-0P, 4-(4-Fluoro-2-methylphenyl)-2-[(trans-4-hydroxycyclohexyl)amino]-8-o-tolyl-8H-pyrido[2,3-d]pyrimidin-7-one 444607-98-1P, 4-(4-Fluoro-2-methylphenyl)-2-((S)-2-hydroxy-1-methylethylamino)-8-o-tolyl-8H-pyrido[2,3-d]pyrimidin-7-one 444608-00-8P, 4-(4-Fluoro-2-methylphenyl)-2-(2-hydroxy-1,1-dimethylethylamino)-8-o-tolyl-8H-pyrido[2,3-d]pyrimidin-7-one 444608-01-9P, 2-Ethylamino-4-(4-fluoro-2-methylphenyl)-8-o-tolyl-8H-pyrido[2,3-d]pyrimidin-7-one 444608-03-1P, 2-Cyclohexylamino-4-(4-fluoro-2-methylphenyl)-8-o-tolyl-8H-pyrido[2,3-d]pyrimidin-7-one 444608-05-3P,  
 4-(4-Fluoro-2-methylphenyl)-2-(tetrahydropyran-4-ylamino)-8-o-tolyl-8H-pyrido[2,3-d]pyrimidin-7-one 444608-07-5P, 4-(4-Fluoro-2-methylphenyl)-8-o-tolyl-2-(2,2,2-trifluoroethylamino)-8H-pyrido[2,3-d]pyrimidin-7-one 444608-08-6P, 4-(4-Fluoro-2-methylphenyl)-2-[(2-hydroxy-1-hydroxymethyl-1-methylethyl)amino]-8-o-tolyl-8H-pyrido[2,3-d]pyrimidin-7-one 444608-11-1P, 2-[[8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-7-oxo-7,8-dihydropyrido[2,3-d]pyrimidine-2-yl]amino]-N,N-dimethylacetamide 444608-13-3P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-[(2-oxo-



methylphenyl)-2-((S)-2-hydroxypropylamino)-8-o-tolyl-8H-pyrido[2,3-d]pyrimidin-7-one 444608-60-0P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-methylamino-8H-pyrido[2,3-d]pyrimidin-7-one 444608-61-1P, 8-(2,6-Difluorophenyl)-2-[[2-(1,1-dioxothiomorpholin-4-yl)-2-oxoethyl]amino]-4-(4-fluoro-2-methylphenyl)-8H-pyrido[2,3-d]pyrimidin-7-one 444608-62-2P, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-[3-(2-oxopyrrolidin-1-yl)propylamino]-8H-pyrido[2,3-d]pyrimidin-7-one 444608-65-5P

, 8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-2-[[2-(5-oxo-4,5-dihydro[1,2,4]oxadiazol-3-yl)ethyl]amino]-8H-pyrido[2,3-d]pyrimidin-7-one 444608-66-6P, 4,8-Bis(2-chlorophenyl)-2-methoxy-8H-pyrido[2,3-d]pyrimidin-7-one 444608-67-7P, 8-(2,6-Difluorophenyl)-4-(2-fluorophenyl)-2-methoxy-8H-pyrido[2,3-d]pyrimidin-7-one 444608-84-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);

THU (Therapeutic use); BIOL (Biological study); PREP

(Preparation); USES (Uses)

(CSBP/p38 kinase inhibitor; preparation of pyridopyrimidinones as CSBP/RK/p38 kinase inhibitors by cyclization reactions of (phenylamino)pyrimidinecarbaldehyde derivs.)

IT 444607-58-3P, 1-[2-[[8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-7-oxo-7,8-dihydropyrido[2,3-d]pyrimidin-2-yl]amino]ethyl]-3-phenylurea 444607-59-4P, 1-[2-[[8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-7-oxo-7,8-dihydropyrido[2,3-d]pyrimidin-2-yl]amino]ethyl]-3-cyclohexylurea 444607-60-7P, 1-[2-[[8-(2,6-Difluorophenyl)-4-(4-fluoro-2-methylphenyl)-7-oxo-7,8-dihydropyrido[2,3-d]pyrimidin-2-yl]amino]ethyl]-3-(3-fluorophenyl)urea 444607-62-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);

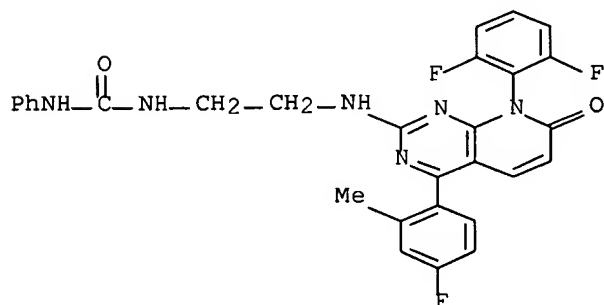
THU (Therapeutic use); BIOL (Biological study); PREP

(Preparation); USES (Uses)

(CSBP/p38 kinase inhibitor; preparation of pyridopyrimidinones as CSBP/RK/p38 kinase inhibitors by cyclization reactions of (phenylamino)pyrimidinecarbaldehyde derivs.)

RN 444607-58-3 HCAPLUS

CN Urea, N-[2-[[8-(2,6-difluorophenyl)-4-(4-fluoro-2-methylphenyl)-7,8-dihydro-7-oxopyrido[2,3-d]pyrimidin-2-yl]amino]ethyl]-N'-phenyl- (CA INDEX NAME)



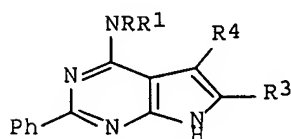
RN 444607-59-4 HCAPLUS

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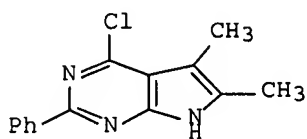
PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 83 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002094974	A1	20020718	US 2000-728616	20001201 <--
US 7160890	B2	20070109		
CA 2430577	A1	20020725	CA 2001-2430577	20011130 <--
WO 2002057267	A1	20020725	WO 2001-US45280	20011130 <--
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BR 2001015847	A	20040225	BR 2001-15847	20011130 <--
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HU 2004000692	A3	20070928		
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			US 1999-169036P	P 19991202 <--
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			US 2000-728316	A 20001201 <--
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			US 2000-728616	A 20001201 <--
			WO 2001-US45280	W 20011130

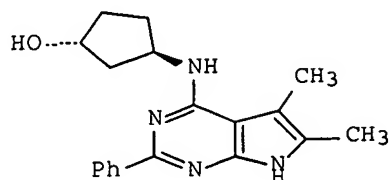
OTHER SOURCE(S): MARPAT 137:109288  
 GI



I



II



III

Lupus erythematosus  
 Mental and behavioral disorders  
 Neoplasm  
 Nervous system, disease  
 Psoriasis  
 Respiratory system, disease  
 Urticaria

(treatment of; preparation of pyrrolo[2,3-d]pyrimidines as selective inhibitors of the adenosine A3 receptor for the treatment of diseases such as diarrhea, allergic rhinitis, and eye damage resulting from injuries or disease)

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	246855-45-8P	246855-46-9P	246855-48-1P	251945-90-1P	251945-91-2P
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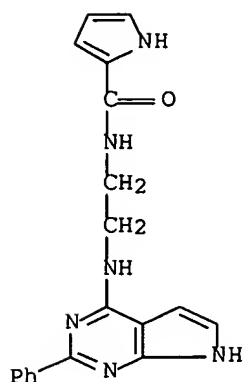
RL: PAC (Pharmacological activity); SPN (Synthetic preparation);  
 THU (Therapeutic use); BIOL (Biological study); PREP  
 (Preparation); USES (Uses)

(invention compound; preparation of pyrrolo[2,3-d]pyrimidines as selective inhibitors of the adenosine A3 receptor for the treatment of diseases such as diarrhea, allergic rhinitis, and eye damage resulting from injuries or disease)

IT 251946-27-7P 343632-15-5P 343632-38-2P  
 443118-41-0P

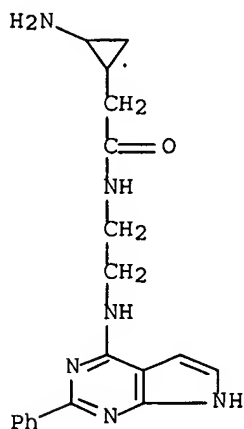
RL: PAC (Pharmacological activity); SPN (Synthetic preparation);  
 THU (Therapeutic use); BIOL (Biological study); PREP  
 (Preparation); USES (Uses)

(invention compound; preparation of pyrrolo[2,3-d]pyrimidines as selective inhibitors of the adenosine A3 receptor for the treatment of diseases such as diarrhea, allergic rhinitis, and eye damage resulting from



RN 443118-41-0 HCAPLUS

CN Cyclopropaneacetamide, 2-amino-N-[2-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 128 THERE ARE 128 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 12 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:536464 HCAPLUS Full-text

DOCUMENT NUMBER: 137:63182

TITLE: Novel bicyclic vitronectin-receptor antagonists, e.g., bicycloheptene and benzazepine derivatives, and their preparation, and pharmaceuticals containing them

INVENTOR(S): Casara, Patrick; Perron, Sierra Francoise; Atassi, Ghanem; Tucker, Gordon; Saint, Dizier Dominique

PATENT ASSIGNEE(S): Adir et Compagnie, Fr.

SOURCE: Fr. Demande, 74 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

50 examples and 25 intermediate preps. are given, with little or no characterizing data. For instance, 5,6,8,9-tetrahydro-7H-benzocyclohepten-7-one (II) was converted in 4 steps to tert-Bu (7-formyl-6,9-dihydro-5H-benzocyclohepten-5-yl)acetate (III). This aldehyde underwent borohydride reduction to an alc., conversion to a bromide, coupling with 2-[(5-hydroxypentyl)amino]pyridine (preparation given), and acid hydrolysis, to give title compound IV.HCl. Compds. I bound to human placental  $\alpha v \beta 3$  and  $\alpha v \beta 5$  vitronectin receptors in vitro with IC50 values on the order of 1 nM. In tests of integrin-dependent cell adhesion using human placental ( $\alpha v \beta 3$ ) and human ovarian carcinoma ( $\alpha v \beta 5$ ) cells, compds. I inhibited adhesion to vitronectin with IC50 values on the order of hundreds of nM and tens of nM, resp. However, in a test for aggregation of platelets from human platelet-rich plasma (side effect), compds. I showed no effect up to 100  $\mu$ M.

IC ICM C07D213-74

ICS C07D235-30; A61K031-4184; A61K031-4402; A61P035-00; A61P009-00

CC 27-21 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1, 25

IT Cardiovascular system, disease

Inflammation

Neoplasm

Osteoporosis

Psoriasis

Rheumatoid arthritis

(treatment; preparation of bicycloheptene and benzazepine derivs. as vitronectin receptor antagonists)

IT 439609-06-0P, tert-Butyl [7-[[[5-(2-pyridinylamino)pentyl]oxy]methyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetate 439609-08-2P, tert-Butyl [7-[[[4-(2-pyridinylamino)butyl]oxy]methyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetate 439609-10-6P, tert-Butyl [7-[[[3-(2-pyridinylamino)propyl]oxy]methyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetate 439609-47-9P, tert-Butyl [7-[[[3-[(2-pyridinylamino)methyl]benzoyl]amino]methyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetate 439609-51-5P, tert-Butyl [7-[[[4-[(N1-4,5,6,7-tetrahydro-3H-azepin-2-yl)amino]butanoyl]amino]methyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetate 439609-53-7P, tert-Butyl [7-[[[4-[(4,5-dihydro-1H-imidazol-2-yl)amino]butanoyl]amino]methyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetate 439609-55-9P, tert-Butyl [7-[[[3-[(1,4,5,6-tetrahydro-2-pyrimidinyl)amino]methyl]benzoyl]amino]methyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetate 439609-58-2P, tert-Butyl [2-Oxo-3-[2-oxo-2-[[3-(2-pyridinylamino)propyl]amino]ethyl]-2,3,4,5-tetrahydro-1H-3-benzazepin-1-yl]acetate 439609-61-7P, tert-Butyl [2-oxo-3-[2-oxo-2-[[4-(2-pyridinylamino)butyl]amino]ethyl]-2,3,4,5-tetrahydro-1H-3-benzazepin-1-yl]acetate 439609-64-0P, tert-Butyl [2-oxo-3-[2-oxo-2-[[2-(2-pyridinylamino)ethyl]amino]ethyl]-2,3,4,5-tetrahydro-1H-3-benzazepin-1-yl]acetate 439609-67-3P, tert-Butyl [2-oxo-3-[2-oxo-2-[[3-[(2-pyridinylamino)methyl]benzyl]amino]ethyl]-2,3,4,5-tetrahydro-1H-3-benzazepin-1-yl]acetate 439609-70-8P, tert-Butyl [2-oxo-3-[2-oxo-2-[[3-[N-(4,5,6,7-tetrahydro-3H-azepin-2-yl)amino]propyl]amino]ethyl]-2,3,4,5-tetrahydro-1H-3-benzazepin-1-yl]acetate 439609-73-1P, tert-Butyl [2-oxo-3-[2-oxo-2-[[3-[(4,5-dihydro-1H-imidazol-2-yl)amino]propyl]amino]ethyl]-2,3,4,5-tetrahydro-1H-3-benzazepin-1-yl]acetate 439609-76-4P, tert-Butyl [2-oxo-3-[2-oxo-2-[[3-[[4,5-dihydro-1H-imidazol-2-yl)amino]methyl]benzyl]amino]ethyl]-2,3,4,5-tetrahydro-1H-3-benzazepin-1-yl]acetate

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; preparation of bicycloheptene and benzazepine derivs. as

[2-Oxo-3-[2-oxo-2-[[3-(2-pyridinylamino)propyl]amino]ethyl]-2,3,4,5-tetrahydro-1H-3-benzazepin-1-yl]acetic acid trifluoroacetate 439609-63-9P, [2-Oxo-3-[2-oxo-2-[[4-(2-pyridinylamino)butyl]amino]ethyl]-2,3,4,5-tetrahydro-1H-3-benzazepin-1-yl]acetic acid trifluoroacetate 439609-66-2P, [2-Oxo-3-[2-oxo-2-[[2-(2-pyridinylamino)ethyl]amino]ethyl]-2,3,4,5-tetrahydro-1H-3-benzazepin-1-yl]acetic acid trifluoroacetate 439609-69-5P, [2-Oxo-3-[2-oxo-2-[[3-[(2-pyridinylamino)methyl]benzyl]amino]ethyl]-2,3,4,5-tetrahydro-1H-3-benzazepin-1-yl]acetic acid trifluoroacetate 439609-72-0P, [2-Oxo-3-[2-oxo-2-[[3-[N-(4,5,6,7-tetrahydro-3H-azepin-2-yl)amino]propyl]amino]ethyl]-2,3,4,5-tetrahydro-1H-3-benzazepin-1-yl]acetic acid trifluoroacetate 439609-75-3P, [2-Oxo-3-[2-oxo-2-[[3-[(4,5-dihydro-1H-imidazol-2-yl)amino]propyl]amino]ethyl]-2,3,4,5-tetrahydro-1H-3-benzazepin-1-yl]acetic acid trifluoroacetate 439609-78-6P, [2-Oxo-3-[2-oxo-2-[[3-[[4,5-dihydro-1H-imidazol-2-yl]amino]methyl]benzyl]amino]ethyl]-2,3,4,5-tetrahydro-1H-3-benzazepin-1-yl]acetic acid trifluoroacetate 439609-79-7P, [7-[[[4-(2-Pyridinylamino)butanoyl]amino]methyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetic acid 439609-80-0P, [7-[[[4-(1H-Benzimidazol-2-ylamino)butanoyl]amino]methyl]-6,9-dihydro-5H-benzocyclohepten-5-yl]acetic acid

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of bicycloheptene and benzazepine derivs. as vitronectin receptor antagonists)

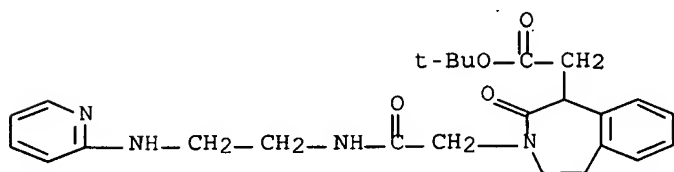
IT 439609-64-0P, tert-Butyl [2-oxo-3-[2-oxo-2-[[2-(2-pyridinylamino)ethyl]amino]ethyl]-2,3,4,5-tetrahydro-1H-3-benzazepin-1-yl]acetate

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; preparation of bicycloheptene and benzazepine derivs. as vitronectin receptor antagonists)

RN 439609-64-0 HCAPLUS

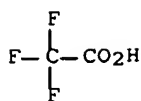
CN 1H-3-Benzazepine-1-acetic acid, 2,3,4,5-tetrahydro-2-oxo-3-[2-oxo-2-[[2-(2-pyridinylamino)ethyl]amino]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



IT 439609-18-4P, [7-[2-Oxo-2-[[2-(2-pyridinylamino)ethyl]amino]ethyl]-5H-benzocyclohepten-5-yl]acetic acid trifluoroacetate 439609-66-2P, [2-Oxo-3-[2-oxo-2-[[2-(2-pyridinylamino)ethyl]amino]ethyl]-2,3,4,5-tetrahydro-1H-3-benzazepin-1-yl]acetic acid trifluoroacetate

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of bicycloheptene and benzazepine derivs. as vitronectin receptor antagonists)



L163 ANSWER 13 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:504782 HCAPLUS Full-text

DOCUMENT NUMBER: 137:78968

TITLE: Preparation of aminocarbonylpyrrolidine derivatives as dipeptidyl peptidase IV inhibitors

INVENTOR(S): Matsuno, Kenji; Ueno, Kimihisa; Iwata, Yasuhiro; Matsumoto, Yuichi; Nakanishi, Satoshi; Takasaki, Kotaro; Kusaka, Hideaki; Nomoto, Yuji; Ogawa, Akira

PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan

SOURCE: PCT Int. Appl., 196 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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RL: PAC (Pharmacological activity); SPN (Synthetic preparation);

THU (Therapeutic use); BIOL (Biological study); PREP

(Preparation); USES (Uses)

(preparation of aminocarbonylpyrrolidine derivs. as dipeptidyl peptidase IV inhibitors)

IT 440101-04-2P 440101-06-4P 440101-07-5P  
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation);

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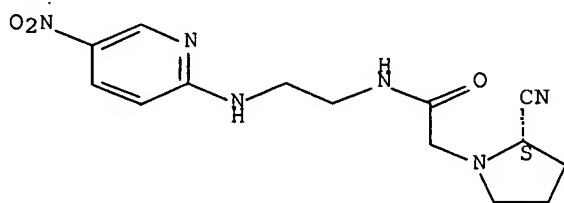
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(preparation of aminocarbonylpyrrolidine derivs. as dipeptidyl peptidase IV inhibitors)

RN 440101-04-2 HCAPLUS

CN 1-Pyrrolidineacetamide, 2-cyano-N-[2-[(5-nitro-2-pyridinyl)amino]ethyl]-,  
(2S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 440101-06-4 HCAPLUS

CN 1-Pyrrolidinecarboxamide, 2-cyano-N-[2-[(5-nitro-2-pyridinyl)amino]ethyl]-,  
(2S)- (CA INDEX NAME)

Absolute stereochemistry.



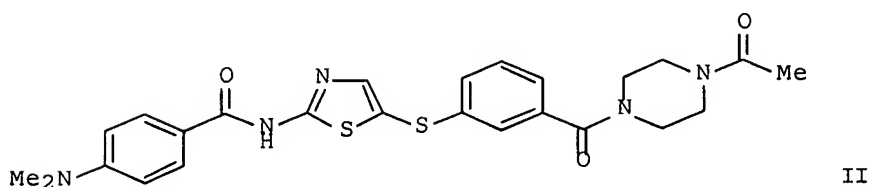
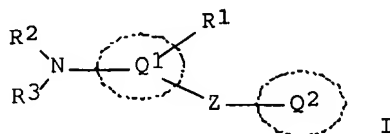
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PRIORITY APPLN. INFO.:

US 2000-257830P	P	20001221 <--
EP 2001-991416	A3	20011219
WO 2001-US49430	W	20011219
US 2001-27982	A3	20011220
US 2003-641535	A1	20030815

OTHER SOURCE(S): MARPAT 137:63240  
 GI



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 439587-28-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);  
 THU (Therapeutic use); BIOL (Biological study); PREP  
 (Preparation); USES (Uses)

(preparation of thiazolyl inhibitors of Tec family tyrosine kinases)

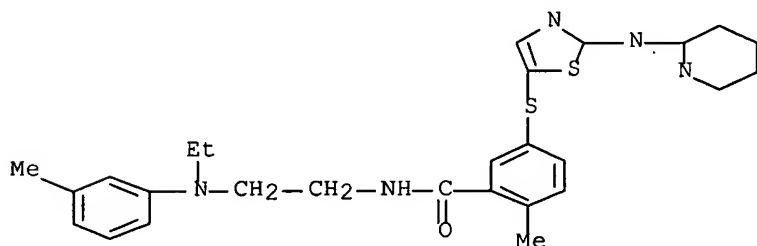
IT 439576-97-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);  
 THU (Therapeutic use); BIOL (Biological study); PREP  
 (Preparation); USES (Uses)

(preparation of thiazolyl inhibitors of Tec family tyrosine kinases)

RN 439576-97-3 HCAPLUS

CN Benzamide, N-[2-[ethyl(3-methylphenyl)amino]ethyl]-2-methyl-5-[[2-(2-pyridinylamino)-5-thiazolyl]thio]- (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 15 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:314939 HCAPLUS Full-text

DOCUMENT NUMBER: 136:340677

TITLE: Preparation of imidazoarenes as antiinflammatory and  
 analgesic agents.

INVENTOR(S): Nakao, Kazunari; Okumura, Yoshiyuki; Matsumizu,  
 Miyako; Uneo, Naomi; Hashizume, Yoshinobu; Kato,  
 Tomoki; Kawai, Akiyoshi; Miyake, Yoriko; Nukui, Seiji;  
 Shinjyo, Katsuhiko; Taniguchi, Kana

PATENT ASSIGNEE(S): Pfizer Pharmaceuticals Inc., Japan; Pfizer Inc.

SOURCE: PCT Int. Appl., 461 pp.

CODEN: PIXXD2

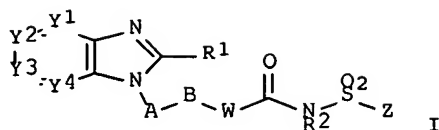
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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AB Title compds. [I; Y1-Y4 = N, CH, CL; R1 = H, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, alkoxy, pyrrolidinyl, amino, etc.; A = (substituted) 5-6 membered monocyclic aromatic ring optionally containing up to 3 heteroatoms selected from O, N, S, etc.; B = halo-substituted alkylene, cycloalkylene, alkenylene, alkynylene, alkyleneoxy, etc., optionally substituted with an oxo group; W = amino, O, S, bond, etc.; R2 = H, OH, alkyl, alkoxy; Z = 5-12 membered (substituted) monocyclic or bicyclic aryl optionally containing up to 3 heteroatoms selected from O, N and S, etc.; L = halo, alkyl, haloalkyl, OH, alkoxy, haloalkoxy, alkylthio, NO<sub>2</sub>, amino, etc.], were prepared as prostaglandin E<sub>2</sub> receptor antagonists, preferably as EP<sub>4</sub> receptor antagonists. Thus, to 2-[4-(2-ethyl-5,7-dimethyl-3H-imidazo[4,5-b]pyridin-3-yl)phenyl]ethylamine (preparation given) in CH<sub>2</sub>Cl<sub>2</sub> was added p-toluenesulfonyl isocyanate followed by stirring for 3 h to give 56% 2-ethyl-5,7-dimethyl-3-[4-[2-[[[(4-methylphenyl)sulfonyl]amino]carbon yl]amino]ethyl]phenyl]-3H-imidazo[4,5-b]pyridine. Preferred I inhibited PGE<sub>2</sub>-induced thermal hyperalgesia in rats with ED<sub>50</sub><60 mg/kg.

IC ICM C07D471-04

ICS A61K031-4178; A61K031-437; A61P029-00; C07D235-08; C07D491-04; C07D473-00; C07D521-00; C07D401-06; C07D401-04; C07D417-12; C07D403-12; C07D401-12; C07D235-30; C07D417-04; C07D403-04; C07D403-06; C07D471-04; C07D235-00; C07D221-00

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

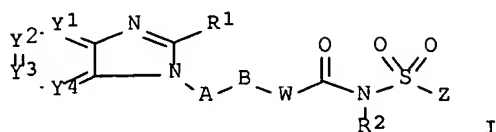
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HU 2003003766	A2	20040428	HU 2003-3766	20011015 <--
AT 320428	T	20060415	AT 2001-978702	20011015 <--
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GI



[2-chloro-4-[(4,6-dimethyl-3-nitro-2-pyridinyl)amino]phenyl]acetate  
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 2-(2-methoxy-4-nitrophenyl)malonate 415912-52-6P, 2-(2-Methoxy-4-nitrophenyl)acetic acid 415912-53-7P, Methyl 2-(2-methoxy-4-nitrophenyl)acetate 415912-54-8P, Methyl 2-(4-amino-2-methoxyphenyl)acetate 415912-55-9P, Methyl [4-[(4,6-dimethyl-3-nitro-2-pyridinyl)amino]-2-methoxyphenyl]acetate 415912-56-0P, Methyl [4-[(3-amino-4,6-dimethyl-2-pyridinyl)amino]-2-methoxyphenyl]acetate 415912-57-1P 415912-58-2P 415912-59-3P 415912-60-6P 415912-61-7P  
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Sakakibara, Sachiko; Yoshino, Takashi; Sato, Hiroki;  
 Masuda, Tsutomu; Koriyama, Yuji; Shimada, Mitsuyuki;  
 Shintani, Takuya; Kadono, Hiroshi; Ziegelbauer, Karl  
 B.; Fuchikami, Kinji; Komura, Hiroshi  
 PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany  
 SOURCE: PCT Int. Appl., 280 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002024679	A1	20020328	WO 2001-EP10405	20010910 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
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BR 2001014073	A	20030617	BR 2001-14073	20010910 <--
EP 1326856	A1	20030716	EP 2001-969704	20010910 <--
EP 1326856	B1	20071219		
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HU 2003003124	A2	20031229	HU 2003-3124	20010910 <--
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US 7232909	B2	20070619		
US 2006205676	A1	20060914	US 2005-240867	20050930 <--
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			NZ 2001-524811	A1 20010910
			WO 2001-EP10405	W 20010910
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OTHER SOURCE(S): MARPAT 136:279345  
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 406211-81-2P 406211-82-3P 406211-83-4P 406211-84-5P 406211-85-6P  
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 406212-30-4P 406212-32-6P 406213-46-5P 406214-93-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);  
 THU (Therapeutic use); BIOL (Biological study); PREP  
 (Preparation); USES (Uses)

(preparation of (hydroxyaryl)pyridines as inhibitors of I $\kappa$ B kinase  
 $\beta$  and as antiinflammatory, immunosuppressant, antitumor, and  
 antiischemic agents)

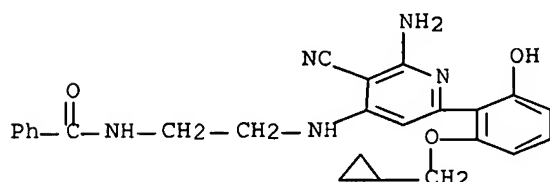
IT 406212-24-6P 406212-26-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);  
 THU (Therapeutic use); BIOL (Biological study); PREP  
 (Preparation); USES (Uses)

(preparation of (hydroxyaryl)pyridines as inhibitors of I $\kappa$ B kinase  
 $\beta$  and as antiinflammatory, immunosuppressant, antitumor, and  
 antiischemic agents)

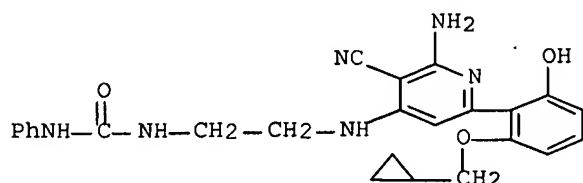
RN 406212-24-6 HCAPLUS

CN Benzamide, N-[2-[[2-amino-3-cyano-6-[2-(cyclopropylmethoxy)-6-  
 hydroxyphenyl]-4-pyridinyl]amino]ethyl]- (CA INDEX NAME)



RN 406212-26-8 HCAPLUS

CN Urea, N-[2-[[2-amino-3-cyano-6-[2-(cyclopropylmethoxy)-6-hydroxyphenyl]-4-  
 pyridinyl]amino]ethyl]-N'-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 18 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:157733 HCAPLUS Full-text

DOCUMENT NUMBER: 136:216541

TITLE: Preparation of novel thioureas as modulators for

AB The title compds. R2YC(:X)NHR1 [X = S, O, NCN; Y = a bond, NR3, O, S; R1 = (un)substituted benzyl, phenethyl, pyridinylmethyl, pyrrolylmethyl, etc.; R2 = (CH2)nR8 (wherein n = 0-4; R8 = CPh, imidazolyl, indolyl, etc.)], useful as modulators for vanilloid receptor (VR), were prepared E.g., a 4-step synthesis of I which showed antagonistic potency 10 times higher than capsazepine in patchclamp test for vanilloid receptor, was given. As diseases associated with the activity of vanilloid receptor, pain acute pain, chronic pain, neuropathic pain, post-operative pain, migraine, arthralgia, neuropathies, nerve injury, diabetic neuropathy, neurodegeneration, neurotic skin disorder, stroke, urinary bladder hypersensitiveness, irritable bowel syndrome, a respiratory disorder such as asthma or chronic obstructive pulmonary disease, irritation of skin, eye or mucous membrane, fervescence, stomach-duodenal ulcer, inflammatory bowel disease and inflammatory diseases can be enumerated. The present invention provides a pharmaceutical composition for prevention or treatment of these diseases.

IC ICM C07C335-16  
ICS C07C311-00; A61K031-00; C07D221-00

CC 25-21 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
Section cross-reference(s): 1, 27, 28

ST thiourea prepn vanilloid receptor analgesic antiinflammatory  
antiulcer; capsaicin receptor thiourea prepn

IT Disease, animal  
Pain  
(arthralgia, treatment of; preparation of novel thioureas as modulators for vanilloid receptor (VR))

IT Nerve, disease  
(neuropathy, treatment of; preparation of novel thioureas as modulators for vanilloid receptor (VR))

IT Analgesics  
Anti-inflammatory agents  
Antiasthmatics  
Antimigraine agents  
Antiulcer agents  
Human  
(preparation of novel thioureas as modulators for vanilloid receptor (VR))

IT 401907-14-0P 401907-15-1P 401907-16-2P 401907-17-3P 401907-18-4P  
401907-19-5P 401907-20-8P 401907-21-9P 401907-22-0P 401907-23-1P  
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 HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,  
 LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,  
 SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,  
 YU, ZA, ZW  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
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 BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
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 EP 1305294 A2 20030502 EP 2001-957342 20010731 <--  
 EP 1305294 B1 20070425  
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 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR  
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 NZ 523774 A 20040924 NZ 2001-523774 20010731 <--  
 AT 360620 T 20070515 AT 2001-957342 20010731 <--  
 ES 2282275 T3 20071016 ES 2001-1957342 20010731 <--  
 NO 2003000473 A 20030130 NO 2003-473 20030130 <--  
 US 2007032653 A1 20070208 US 2003-333556 20031020 <--  
 PRIORITY APPLN. INFO.: US 2000-222584P P 20000801 <--  
 WO 2001-US23959 W 20010731  
 OTHER SOURCE(S): MARPAT 136:167373  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Imidazole derivs. I [R1 = H, (CH<sub>2</sub>)<sub>m</sub>CO(CH<sub>2</sub>)<sub>m</sub>Z1, (CH<sub>2</sub>)<sub>m</sub>Z1, etc.; Z1 = (un)substituted benzo[b]thiophene, Ph, naphthyl, etc.; m = 0-6; R2 = H, alkyl; R1 and R2 taken together with the nitrogen atoms to which they are attached form II-IV; R3 = (CH<sub>2</sub>)<sub>m</sub>E(CH<sub>2</sub>)<sub>m</sub>Z2; E = O, S, CO, etc.; Z2 = H, alkyl, NH<sub>2</sub>, etc.; R4 = H, (CH<sub>2</sub>)<sub>m</sub>A1; A1 = C(:Y)NX1X2; C(:Y)X2; C(:NH)X2, X2; Y = O, S; X1 = H, alkyl, etc.; X2 = alkyl, etc.; R5 = alkyl, (un)substituted aryl, etc.; R6 = H, alkyl; R7 = alkyl, (CH<sub>2</sub>)<sub>m</sub>Z4; Z4 = (un)substituted Ph, naphthyl, indolyl, etc.], which are useful as agonists or antagonists of somatostatin receptors (no data) and for inhibiting the proliferation of Helicobacter pylori, were prepared. Thus, activating 2-furancarboxylic acid with carbonyldiimidazole followed by addition of 2-{(1S)-1-amino-2-(indol-3-yl)ethyl}-4-phenyl-1H-imidazole afforded 94% the title compound V. Compds. I are effective at 0.01-10.0 mg/kg/day.

IC ICM C07D233-54  
 ICS C07D403-06; A61P005-02

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1

IT Nerve, disease  
 (diabetic neuropathy; preparation of imidazolyl derivs. as agonists or antagonists of somatostatin receptors)

IT 167983-80-4P 175531-38-1P 252279-11-1P 252279-15-5P 252292-70-9P  
 252292-71-0P 252292-72-1P 252292-73-2P 252292-74-3P 252292-75-4P  
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252297-69-1P				

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);  
 THU (Therapeutic use); BIOL (Biological study); PREP  
 (Preparation); USES (Uses)

(preparation of imidazolyl derivs. as agonists or antagonists of  
 somatostatin receptors)

IT 252294-89-6P 252295-88-8P 252295-89-9P  
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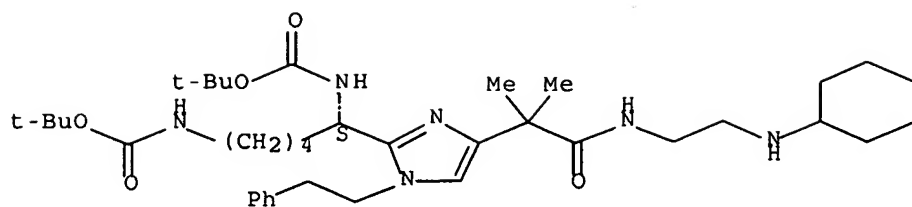
RL: PAC (Pharmacological activity); SPN (Synthetic preparation);  
 THU (Therapeutic use); BIOL (Biological study); PREP  
 (Preparation); USES (Uses)

(preparation of imidazolyl derivs. as agonists or antagonists of  
 somatostatin receptors)

RN 252294-89-6 HCAPLUS

CN Carbamic acid, [(1S)-1-[1-(4-bromophenyl)-4-[2-[[2-(cyclohexylamino)ethyl]amino]-1,1-dimethyl-2-oxoethyl]-1H-imidazol-2-yl]-1,5-pentanediy]]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

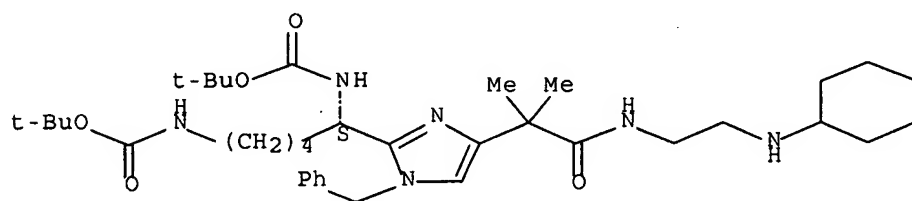
Absolute stereochemistry.



RN 252295-91-3 HCAPLUS

CN Carbamic acid, [(1S)-1-[4-[2-[[2-(cyclohexylamino)ethyl]amino]-1,1-dimethyl-2-oxoethyl]-1-(phenylmethyl)-1H-imidazol-2-yl]-1,5-pentanediy]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

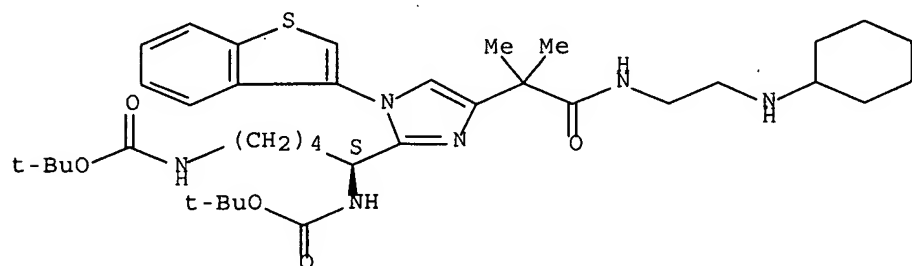
Absolute stereochemistry.



RN 252295-92-4 HCAPLUS

CN Carbamic acid, [(1S)-1-[1-benzo[b]thien-3-yl-4-[2-[[2-(cyclohexylamino)ethyl]amino]-1,1-dimethyl-2-oxoethyl]-1H-imidazol-2-yl]-1,5-pentanediy]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

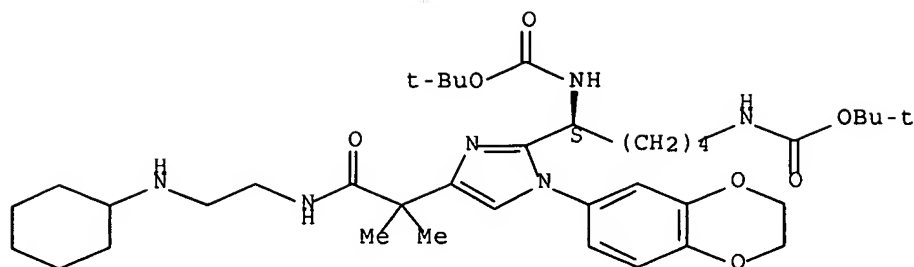
Absolute stereochemistry.



RN 252295-93-5 HCAPLUS

CN Carbamic acid, [(1S)-1-[4-[2-[[2-(cyclohexylamino)ethyl]amino]-1,1-dimethyl-2-oxoethyl]-1-(4-nitrophenyl)-1H-imidazol-2-yl]-1,5-pentanediy]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

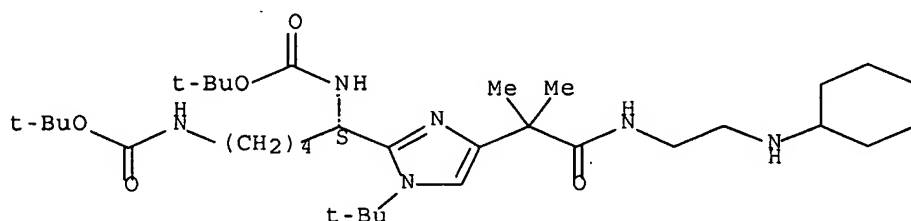
Absolute stereochemistry.



RN 252295-97-9 HCAPLUS

CN Carbamic acid, [(1S)-1-[4-[2-[[2-(cyclohexylamino)ethyl]amino]-1,1-dimethyl-2-oxoethyl]-1-(1,1-dimethylethyl)-1H-imidazol-2-yl]-1,5-pentanediy]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L163 ANSWER 20 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:886087 HCAPLUS Full-text

DOCUMENT NUMBER: 136:20063

TITLE: Preparation of aminocyclohexylbenzazolonones as NMDA receptor antagonists.

INVENTOR(S): Nikam, Sham Shridhar; Scott, Ian Leslie; Sherer, Brian Alan; Wise, Lawrence David

PATENT ASSIGNEE(S): Warner-Lambert Company, USA

SOURCE: PCT Int. Appl., 156 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001092239	A1	20011206	WO 2001-US14763	20010508 <--
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
CA 2409006	A1	20011206	CA 2001-2409006	20010508 <--

377083-35-7P 377083-37-9P 377083-39-1P 377083-41-5P

377083-45-9P 377083-47-1P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN

(Synthetic preparation); THU (Therapeutic use); BIOL (Biological

study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of aminocyclohexylbenzazolones as NMDA receptor antagonists)

IT 377082-67-2P 377082-68-3P 377082-70-7P 377082-72-9P 377082-73-0P  
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation);

THU (Therapeutic use); BIOL (Biological study); PREP

(Preparation); USES (Uses)

(preparation of aminocyclohexylbenzazolones as NMDA receptor antagonists)

IT 1811-85-4P 5797-82-0P 19932-85-5P 27650-80-2P 32190-97-9P  
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)

(preparation of aminocyclohexylbenzazolones as NMDA receptor antagonists)

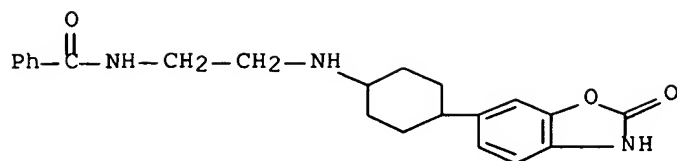
IT 377083-45-9P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN

(Synthetic preparation); THU (Therapeutic use); BIOL (Biological

study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of aminocyclohexylbenzazolones as NMDA receptor antagonists)



● HCl

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 21 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2001:730700 HCAPLUS Full-text  
 DOCUMENT NUMBER: 135:288686  
 TITLE: Synthesis of substituted N-acyl/sulfonyl pyrrolidine derivatives as bax inhibitors  
 INVENTOR(S): Halazy, Serge; Schwarz, Matthias; Quattropani, Anna; Thomas, Russel; Baxter, Anthony; Scheer, Alexander  
 PATENT ASSIGNEE(S): Applied Research Systems ARS Holding N.V., Neth. Antilles  
 SOURCE: PCT Int. Appl., 219 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001072705	A1	20011004	WO 2001-EP3171	20010320 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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EP 1268419	A1	20030102	EP 2001-929439	20010320 <--
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BR 2001009900	A	20030603	BR 2001-9900	20010320 <--
HU 2003000994	A2	20030828	HU 2003-994	20010320 <--
JP 2003528854	T	20030930	JP 2001-570618	20010320 <--
NZ 521060	A	20040528	NZ 2001-521060	20010320 <--
EE 200200555	A	20040615	EE 2002-555	20010320 <--
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ZA 2002006799	A	20030826	ZA 2002-6799	20020826 <--
IN 2002MN01184	A	20040605	IN 2002-MN1184	20020828 <--
BG 107132	A	20030430	BG 2002-107132	20020923 <--
NO 2002004598	A	20021125	NO 2002-4598	20020925 <--

(premature; synthesis of substituted N-acyl/sulfonyl pyrrolidine  
derivs. as bax inhibitors)

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365456-73-1P 365456-76-4P 365456-78-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug; synthesis of substituted N-acyl/sulfonyl pyrrolidine derivs. as bax inhibitors)

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365456-76-4P 365456-78-6P

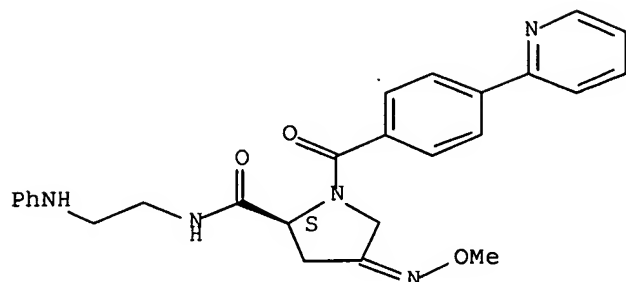
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug; synthesis of substituted N-acyl/sulfonyl pyrrolidine derivs. as bax inhibitors)

RN 365456-63-9 HCAPLUS

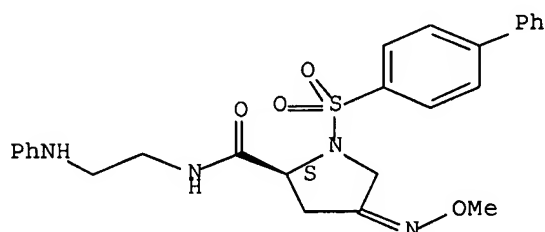
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Absolute stereochemistry.  
Double bond geometry unknown.



RN 365456-78-6 HCAPLUS  
CN 2-Pyrrolidinecarboxamide, 1-([1,1'-biphenyl]-4-ylsulfonyl)-4-(methoxyimino)-N-[2-(phenylamino)ethyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry unknown.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 22 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2001:713354 HCAPLUS Full-text  
DOCUMENT NUMBER: 135:272895  
TITLE: Preparation of Furanoisoquinoline derivatives as phosphodiesterase IV inhibitors  
INVENTOR(S): Kawano, Yasuhiko; Matsumoto, Tatsumi; Uchikawa, Osamu; Fujii, Nobuhiro; Tarui, Naoki  
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., USA  
SOURCE: PCT Int. Appl., 620 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001070746	A1	20010927	WO 2001-JP2277	20010322 <--
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Autoimmune disease  
Cholinergic antagonists  
Diabetes insipidus  
Diabetes mellitus  
Rheumatoid arthritis

(preparation of furano-isoquinoline derivs. as phosphodiesterase IV inhibitors)

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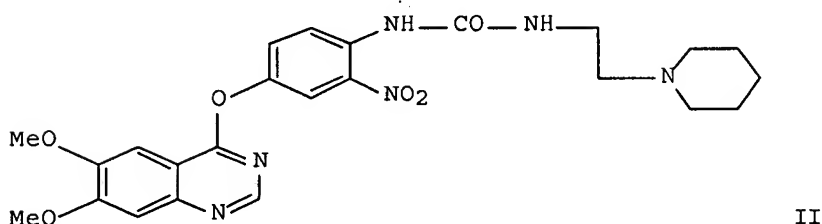
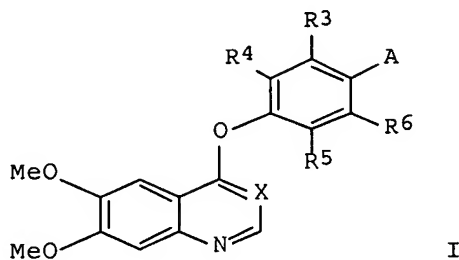
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of furano-isoquinoline derivs. as phosphodiesterase IV inhibitors)

IT 362709-34-0P 362709-35-1P

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OTHER SOURCE(S):      MARPAT 135:92649  
 GI



AB Title compds. [I; X = N, CH; R3, R4, R5, R6 independently = H, Cl, F, CH3, CH3O, NO2; A = 4-CH3C6H4CH2OCONH, 3-ClC6H4CH(CH3)OCONH, 4-FC6H4CH2OCONH, 2-ClC6H4CH(CH3)OCONH, 2-ClC6H4CH2CH2CH2OCONH, 4- CF3C6H4CH2OCONH, CH3(CH2)5OCONH, (CH3CH2)2N(CH2)3NHCSNH, YNHCONH, 4-ClC6H4O(CH2)2S, 4-ClC6H4(CH2)2NH, 3-BrC6H4CONHCSNH, C6H5COO, OH, OCH2COOCH3, OCH2COOH; Y = heterocycle, heterocyclylalkyl] and pharmaceutically acceptable salts are prepared as remedies for diseases mediated by autophosphorylation of PDGF receptors, particularly useful as intimal thickening inhibitors. Thus, the title claimed compound II was prepared and biol. tested.

IC ICM C07D215-233

347156-79-0P 347156-80-3P 347156-81-4P 347156-82-5P 347156-83-6P

347156-84-7P 347156-85-8P

RL: BAC (Biological activity or effector, except adverse); BSU  
(Biological study, unclassified); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(preparation of quinazolines and quinolines as remedies for diseases  
mediated by autophosphorylation of PDGF receptors)

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347156-21-2P 347156-22-3P 347156-23-4P  
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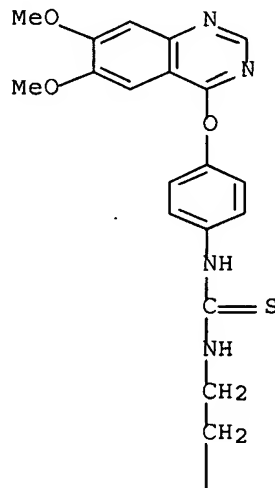
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(Biological study, unclassified); SPN (Synthetic preparation); THU  
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(Uses)

(preparation of quinazolines and quinolines as remedies for diseases  
mediated by autophosphorylation of PDGF receptors)

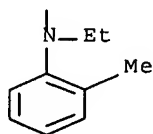
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PAGE 1-A



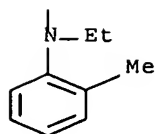
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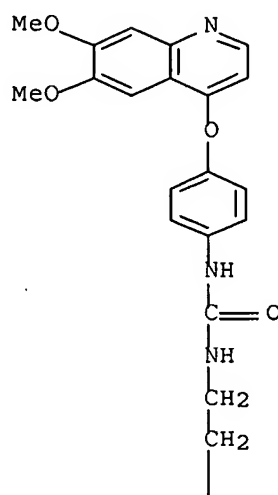
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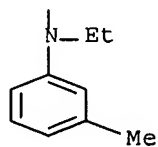
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PAGE 1-A



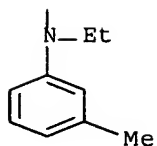
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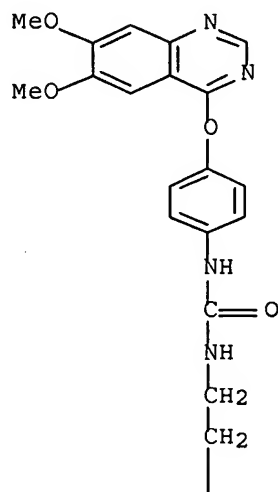
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PAGE 2-A

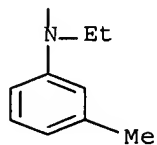


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PAGE 1-A

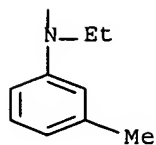


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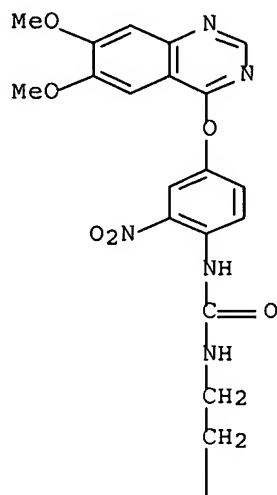
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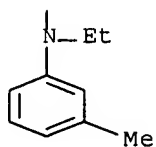
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PAGE 1-A



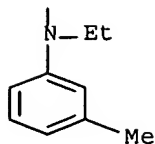
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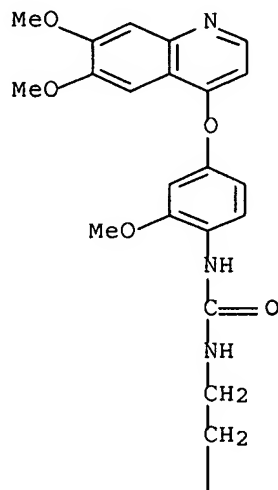
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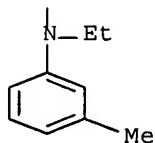


RN 347156-30-3 HCAPLUS  
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PAGE 1-A



PAGE 2-A



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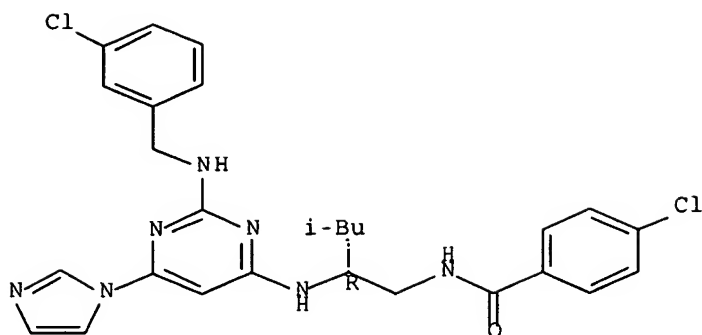
L163 ANSWER 24 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2001:63992 HCAPLUS Full-text  
 DOCUMENT NUMBER: 134:116237  
 TITLE: Preparation of bradykinin B1 receptor antagonists  
 INVENTOR(S): Ohlmeyer, Michael H. J.; Baldwin, John J.; Dolle, Roland E., III; Paradkar, Vidyadhar; Quintero, Jorge

Section cross-reference(s): 1, 28, 63

- IT Pain  
(hyperalgesia; preparation of bradykinin B1 receptor antagonists)
- IT Alopecia  
Alzheimer's disease  
Analgesics  
Anti-inflammatory agents  
Antiasthmatics  
Atherosclerosis  
Diuresis  
Edema  
Hyperglycemia  
Liver, disease  
Multiple sclerosis  
(preparation of bradykinin B1 receptor antagonists)
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(Reactant or reagent)  
(preparation of bradykinin B1 receptor antagonists)
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(preparation of bradykinin B1 receptor antagonists)
- IT 321328-74-9P 321329-69-5P 321329-71-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation of bradykinin B1 receptor antagonists)
- RN 321328-74-9 HCAPLUS
- CN Benzamide, 4-chloro-N-[(2R)-2-[[2-chloro-6-(1H-imidazol-1-yl)-4-pyrimidinyl]amino]-4-methylpentyl]- (CA INDEX NAME)

Absolute stereochemistry.

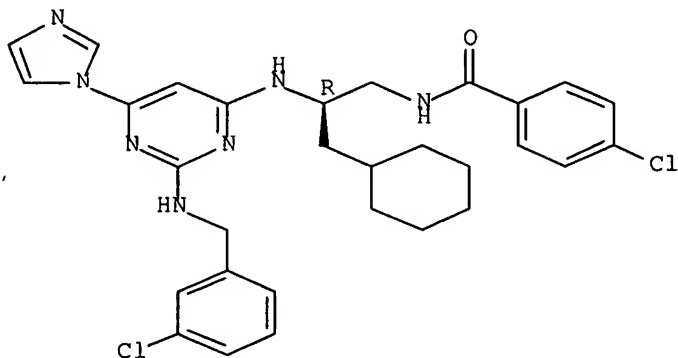




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Absolute stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 25 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:31510 HCAPLUS Full-text

DOCUMENT NUMBER: 134:100882

TITLE: Thieno- and furopyrimidine derivatives as a2a-receptor antagonists

INVENTOR(S): Gillespie, Roger John; Giles, Paul Richard; Lerpinriere, Joanne; Dawson, Claire Elizabeth; Bebbington, David

PATENT ASSIGNEE(S): Vernalis Research Limited, UK

SOURCE: PCT Int. Appl., 88 pp.

CODEN: PIXXD2.

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001002409	A1	20010111	WO 2000-GB2517	20000630 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				

ICS C07D491-04; A61K031-505; A61P025-14; C07D495-04; C07D333-00;  
C07D239-00

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

IT Alzheimer's disease

Movement disorders

Pain

Parkinson's disease

Wilson's disease

(preparation of thieno[3,2-d]pyrimidine and furo[3,2-d]pyrimidine derivs.

as

adenosine A2a receptor antagonists for the treatment of movement disorders such as Parkinson's disease)

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RL: BAC (Biological activity or effector, except adverse); BSU  
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(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

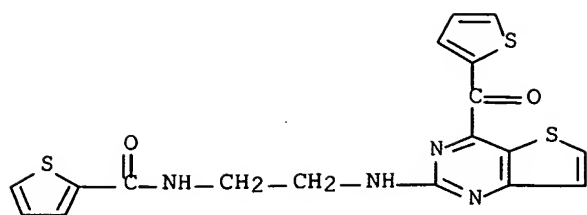
(preparation of thieno[3,2-d]pyrimidine and furo[3,2-d]pyrimidine derivs.

as

adenosine A2a receptor antagonists for the treatment of movement disorders such as Parkinson's disease)

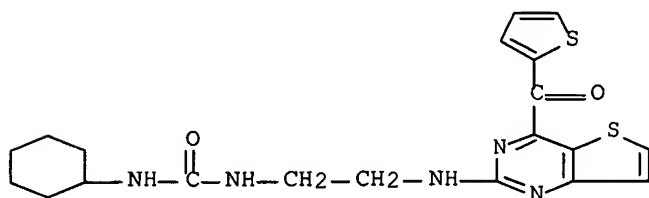
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RL: BAC (Biological activity or effector, except adverse); BSU



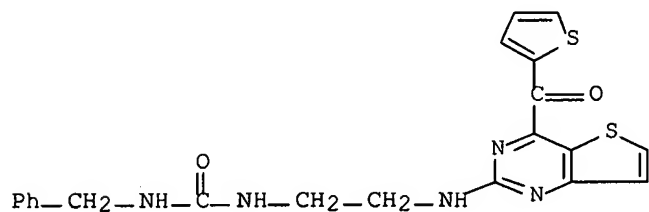
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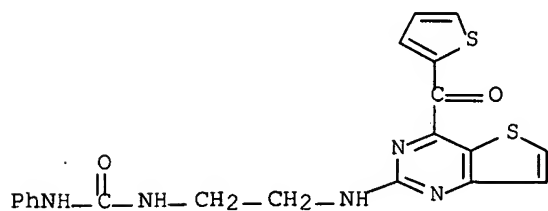
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CN Urea, N-phenyl-N'-[2-[[4-(2-thienylcarbonyl)thieno[3,2-d]pyrimidin-2-yl]amino]ethyl]- (CA INDEX NAME)



RN 319442-08-5 HCAPLUS

CN Urea, N-(4-chlorophenyl)-N'-[2-[[4-(2-thienylcarbonyl)thieno[3,2-d]pyrimidin-2-yl]amino]ethyl]- (CA INDEX NAME)

## RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 26 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:881130 HCAPLUS Full-text

DOCUMENT NUMBER: 134:42124

TITLE: Preparation of diaminothiazoles for inhibiting protein kinases

INVENTOR(S): Chu, Shao Song; Alegria, Larry Andrew; Bender, Steven Lee; Benedict, Suzanne Pritchett; Borchardt, Allen J.; Kania, Robert Steve; Nambu, Mitchell David; Tempczyk-Russell, Anna Maria; Sarshar, Sepehr

PATENT ASSIGNEE(S): Agouron Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 397 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000075120	A1	20001214	WO 2000-US15188	20000602 <--
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OTHER SOURCE(S): MARPAT 134:42124

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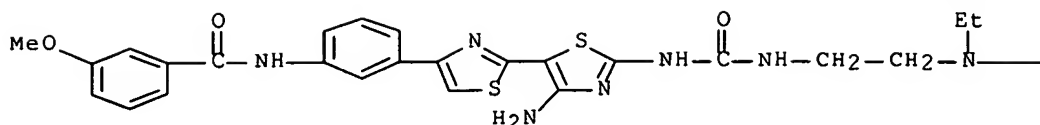
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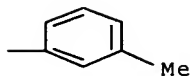
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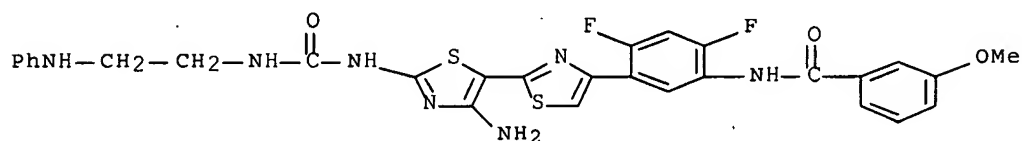


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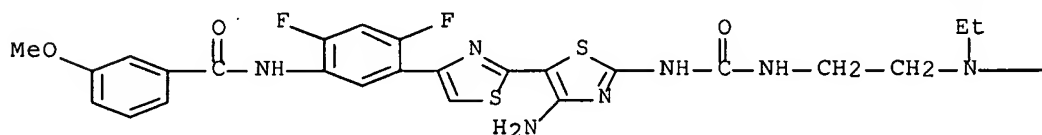
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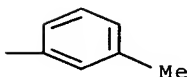
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PAGE 1-A



PAGE 1-B



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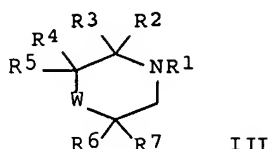
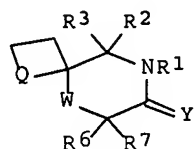
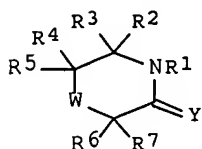
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INDEX NAME)

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EP 1140876	A1	20011010	EP 1999-966439	19991217 <--
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US 2002068737	A1	20020606	US 2001-17263	20011214 <--
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OTHER SOURCE(S):                    MARPAT 133:58807

GI



AB Title compds. [I; II; III; W = O, S, NR8; R8 = H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl; Y = O, S; R1 = specified (substituted) piperidinylalkylaminocarbonyl, piperazinylalkylaminocarbonyl, etc.; R2 = (substituted) aryl, heteroaryl; R3 = H, alkyl, fluoroalkyl, polyfluoroalkyl; R4-R7 = H, (CH2)tYR8, (CH2)tCO2R8, (CH2)tCN, alkyl, alkenyl, alkynyl, cycloalkyl, (substituted) Ph, PhCH2, etc.; Q = (CH2)0-4; Y = O, S], were prepared. Thus, (+)-3-(3,4-difluorophenyl)-5-oxomorpholine-4-carboxylic acid 4-nitrophenyl ester (preparation given) and 3-[4-(5-fluoro-2-methoxyphenyl)-4-phenylpiperidin-1-yl]propylamine were stirred at room temperature overnight in THF to give (+)-3-(3,4-difluorophenyl)-5-oxomorpholine-4-carboxylic acid 3-[4-(5-fluoro-2-methoxyphenyl)-4-phenylpiperidin-1-yl]propylamide. The latter bound to human  $\alpha_1$  receptors with  $K_i = 1.6$  nM.

IC ICM C07D265-32

ICS C07D413-12; A01N031-5377; A01N031-5375

CC 28-13 (Heterocyclic Compounds (More Than One Hetero Atom))

ST morpholine carbamoyl prepn adrenergic antagonist; benign prostatic hypertrophy treatment carbamoylmorpholine prepn; intraocular antihypertensive carbamoylmorpholine prepn; migraine treatment carbamoylmorpholine prepn; analgesic carbamoylmorpholine prepn; antiarrhythmic carbamoylmorpholine prepn

IT Analgesics

Antiarrhythmics

Anticholesteremic agents

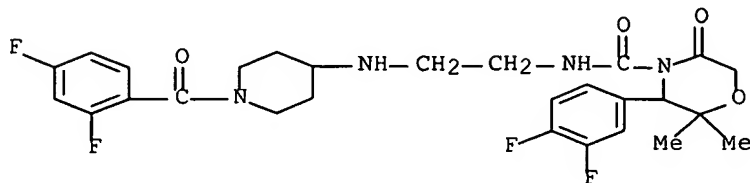
Antiglaucoma agents

Antimigraine agents

(preparation of morpholine derivs: as selective antagonists of  $\alpha_1$  receptors)

IT 277295-67-7P 277295-68-8P 277295-70-2P 277295-72-4P 277295-73-5P  
277295-74-6P 277295-75-7P 277295-76-8P 277295-77-9P

RN 277295-88-2 HCAPLUS  
 CN 4-Morpholinecarboxamide, N-[2-[[1-(2,4-difluorobenzoyl)-4-piperidinyl]amino]ethyl]-3-(3,4-difluorophenyl)-2,2-dimethyl-5-oxo- (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 28 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1999:659372 HCAPLUS Full-text  
 DOCUMENT NUMBER: 131:286397  
 TITLE: Preparation of fused thiophene derivatives as interleukin-6 and interleukin-12 production inhibitors  
 INVENTOR(S): Konishi, Mikio; Katsube, Nobuo; Konno, Mitoshi; Kishimoto, Tadimitsu  
 PATENT ASSIGNEE(S): Ono Pharmaceutical Co., Ltd., Japan  
 SOURCE: PCT Int. Appl., 717 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9951587	A1	19991014	WO 1999-JP1648	19990331 <--
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RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9930531	A	19991025	AU 1999-30531	19990331 <--
EP 1067128	A1	20010110	EP 1999-912051	19990331 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
US 6420391	B1	20020716	US 2000-647430	20001002 <--
US 2003073706	A1	20030417	US 2002-127409	20020423 <--
US 6555555	B1	20030429		
PRIORITY APPLN. INFO.:			JP 1998-104210	A 19980401 <--
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OTHER SOURCE(S):			MARPAT 131:286397	
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RL: BAC (Biological activity or effector, except adverse); BSU  
(Biological study, unclassified); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(preparation of fused thiophene derivs. as interleukin-6 and interleukin-12  
production inhibitors)

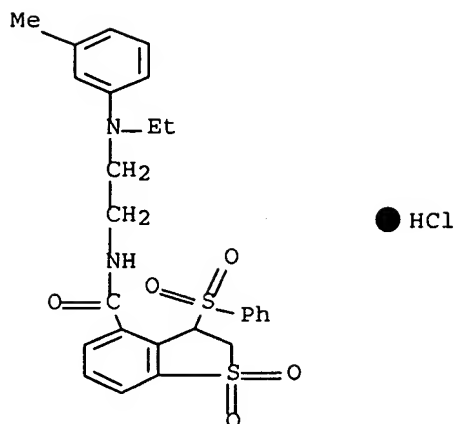
IT 246175-66-6P 246175-83-7P 246175-84-8P

RL: BAC (Biological activity or effector, except adverse); BSU  
(Biological study, unclassified); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(preparation of fused thiophene derivs. as interleukin-6 and interleukin-12  
production inhibitors)

RN 246175-66-6 HCAPLUS

CN Benzo[b]thiophene-4-carboxamide, N-[2-[ethyl(3-methylphenyl)amino]ethyl]-,  
1,1-dioxide (CA INDEX NAME)



REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 29 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1999:126886 HCAPLUS Full-text  
 DOCUMENT NUMBER: 130:196584  
 TITLE: Preparation of aniline derivatives as calcium channel blockers  
 INVENTOR(S): Hu, Lain-Yen; Rafferty, Michael Francis; Ryder, Todd Robert  
 PATENT ASSIGNEE(S): Warner-Lambert Company, USA  
 SOURCE: PCT Int. Appl., 137 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9907689	A1	19990218	WO 1998-US15907	19980729 <--
W: AL, AU, BA, BB, BG, BR, CA, CN, CZ, EE, GE, HR, HU, ID, IL, IS, JP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9887627	A	19990301	AU 1998-87627	19980729 <--
ZA 9807144	A	19990510	ZA 1998-7144	19980807 <--
US 6251918	B1	20010626	US 1999-402196	19990929 <--
US 2001023249	A1	20010920	US 2001-769798	20010125 <--
US 6495715	B2	20021217		
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			US 1998-82358P	P 19980420 <--
			WO 1998-US15907	W 19980729 <--
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			US 2001-769798	A3 20010125

OTHER SOURCE(S): MARPAT 130:196584  
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RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(preparation of aniline derivs. as calcium channel blockers)

IT 220737-47-3P 220738-18-1P

RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(preparation of aniline derivs. as calcium channel blockers)

RN 220737-47-3 HCAPLUS

CN Pentanamide, 2-(2-cyclohexen-1-ylmethylamino)-N-[1,1-dimethyl-2-[(3-methyl-  
 3-butenyl) [4-(phenylmethoxy)phenyl]amino]ethyl]-4-methyl-, (2S)- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.

W: AM, AT, AU, AZ, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB,  
HU, JP, KG, KR, KZ, LT, LU, LV, MD, MX, NO, NZ, PL, PT, RO, RU,  
SE, SG, SI, SK, TJ, TM, UA, VN

RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

AU 9660243 A 19961218 AU 1996-60243 19960530 <--

AU 723577 B2 20000831

EP 832076 A1 19980401 EP 1996-917833 19960530 <--

EP 832076 B1 20030716

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
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CN 1202893 A 19981223 CN 1996-195931 19960530 <--

JP 11504651 T 19990427 JP 1996-536579 19960530 <--

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HU 9900102 A3 20011128

BR 9609151 A 19990629 BR 1996-9151 19960530 <--

AT 245150 T 20030815 AT 1996-917833 19960530 <--

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ZA 9604486 A 19971201 ZA 1996-4486 19960531 <--

TW 454007 B 20010911 TW 1996-85107183 19960614 <--

LT 4416 B 19981228 LT 1997-182 19971124 <--

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US 1994-232961 B2 19940422 <--

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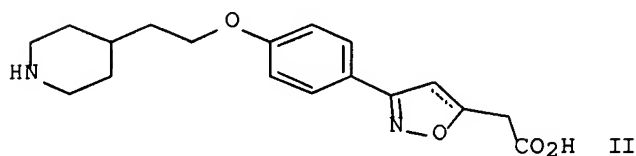
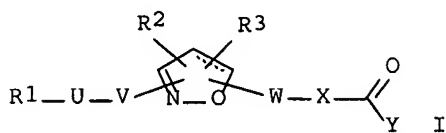
NZ 1994-276633 A1 19941114 <--

US 1995-455436 A 19950531 <--

WO 1996-US7692 W 19960530 <--

OTHER SOURCE(S): MARPAT 130:66484

GI



AB The invention relates to novel isoxazolines and isoxazoles which are useful as antagonists of the platelet glycoprotein IIb/IIIa fibrinogen receptor complex or the vitronectin receptor. The invention also relates to pharmaceutical compns. containing the compds., processes for preparing the compds., and to methods of using these compds., alone or in combination with other therapeutic agents, for the inhibition of platelet aggregation, as thrombolytics, and/or for the treatment of thromboembolic disorders. Such disorders include

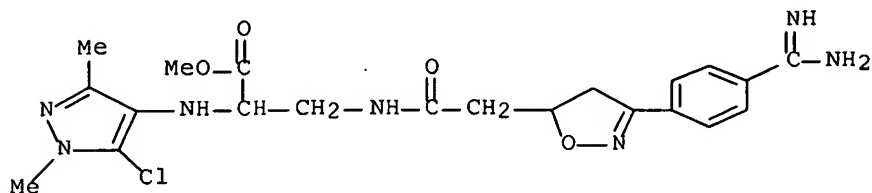
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RL: BAC (Biological activity or effector, except adverse); BSU  
(Biological study, unclassified); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(preparation of novel isoxazoline and isoxazole fibrinogen receptor  
antagonists)

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RN 185967-17-3 HCAPLUS  
 CN Alanine, 3-[[[3-[4-(aminoiminomethyl)phenyl]-4,5-dihydro-5-isoxazolyl]acetyl]amino]-N-(5-chloro-1,3-dimethyl-1H-pyrazol-4-yl)-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 31 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1998:527309 HCAPLUS Full-text  
 DOCUMENT NUMBER: 129:148822  
 TITLE: Preparation and formulation of aminobenzophenones as inhibitors of interleukin and TNF  
 INVENTOR(S): Ottosen, Erik Rytter; Rachlin, Schneur  
 PATENT ASSIGNEE(S): Leo Pharmaceutical Products Ltd. A/S (Lovens Kemiske Fabrik Produktionsaktie, Den.  
 SOURCE: PCT Int. Appl., 81 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

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RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(preparation of aminobenzophenones as inhibitors of interleukin and TNF)

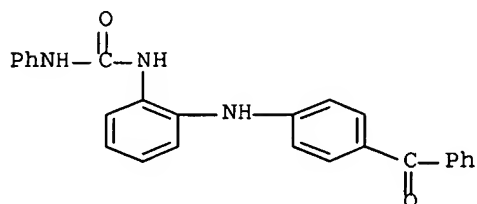
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RL: BAC (Biological activity or effector, except adverse); BSU  
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(preparation of aminobenzophenones as inhibitors of interleukin and TNF)

RN 210965-94-9 HCAPLUS

CN Urea, N-[2-[(4-benzoylphenyl)amino]phenyl]-N'-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L163 ANSWER 32 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:479029 HCAPLUS Full-text

DOCUMENT NUMBER: 129:122458

TITLE: Preparation of N,N'-diphenylurea derivatives as interleukin-8 receptor antagonists

INVENTOR(S): Widdowson, Katherine Louisa; Veber, Daniel Frank; Jurewicz, Anthony Joseph; Hertzberg, Robert Philip; Rutledge, Melvin Clarence, Jr.

PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA

SOURCE: U.S., 50 pp., Cont.-in-part of U.S. Ser. No. 641,990.  
 CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 5

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RL: BAC (Biological activity or effector, except adverse); BSU  
(Biological study, unclassified); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(preparation of N,N'-diphenylurea derivs. as interleukin-8 receptor  
antagonists for disease treatment)

IT 182498-76-6P

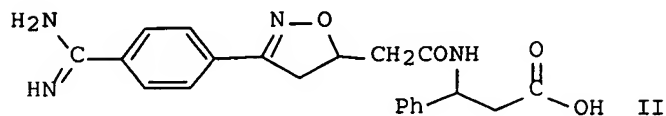
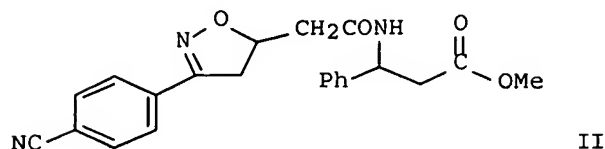
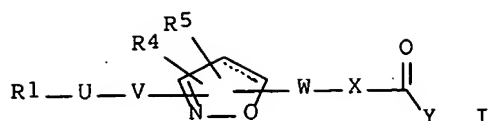
RL: BAC (Biological activity or effector, except adverse); BSU  
(Biological study, unclassified); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(preparation of N,N'-diphenylurea derivs. as interleukin-8 receptor  
antagonists for disease treatment)

RN 182498-76-6 HCAPLUS

CN Urea, N-(2-hydroxy-4-nitrophenyl)-N'-[2-(phenylamino)phenyl]- (CA INDEX  
NAME)





AB The title compds. [I; R1 = R2NR3(CH2)qZ- (wherein R2, R3 = H, C1-10 alkyl, C2-6 alkenyl, etc.; Z O, S, SO, SO2, etc.; q = 2-7), piperazinyl(CH2)qZ-, etc.; U = a single bond, C1-7 alkyl, C2-7 alkenyl, etc.; V = a single bond, (un)substituted C1-7 alkyl, etc.; W = a single bond, C1-7 alkyl, C2-7 alkenyl, etc.; X = a single bond, (un)substituted C1-7 alkyl, etc.; Y = OH, C1-10 alkoxy, etc.; R4 = H, C1-10 alkyl, C2-10 alkenyl, etc.; R5 = H, (un)substituted C1-10 alkyl, C2-10 alkenyl, etc.], useful alone or in combination with other therapeutic agents, for the inhibition of platelet aggregation, as thrombolytics, and/or for the treatment of thromboembolic disorders selected from, e.g. restenosis, atherosclerosis, stroke, myocardial infarction, and unstable angina, were prepared and formulated. Thus, reaction of Me 3-(3-butenoyl)amino-3-phenylpropionate with 4-cyanobenzaldoxime in CH2Cl2 in the presence of 5% NaOCl (aqueous) followed by treatment of the intermediate II in 10% DCM/MeOH with gaseous HCl, addition of (NH4)2CO3 to the crude imidate in MeOH, and saponification afforded III which showed IC50 of <10  $\mu$ M against platelet aggregation. Compds. I are useful also for treating rheumatoid arthritis, asthma, allergies, organ transplantation rejection, septic shock, psoriasis, contact dermatitis, osteoporosis, osteoarthritis, tumor metastasis, diabetic retinopathy, and inflammatory conditions.

IC ICM C07D261-04

ICS A61K031-42; C07D261-10; C07D498-10; C07D413-04; C07D413-10;  
C07D413-06; C07D413-14; C07D413-12

CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 63

ST fibrinogen receptor antagonist isoxazoline isoxazole prepn; thrombosis isoxazoline isoxazole prepn; platelet aggregation inhibitor isoxazoline isoxazole prepn; restenosis isoxazoline isoxazole prepn; antiatherosclerotic isoxazoline isoxazole prepn; stroke isoxazoline isoxazole prepn; myocardial infarction isoxazoline isoxazole prepn; angina isoxazoline isoxazole prepn; rheumatoid arthritis isoxazoline isoxazole prepn; antiasthmatic isoxazoline isoxazole prepn; allergy inhibitor isoxazoline isoxazole prepn; organ transplantation rejection isoxazoline isoxazole prepn; septic shock isoxazoline isoxazole prepn; psoriasis isoxazoline isoxazole prepn; contact dermatitis isoxazoline isoxazole prepn; osteoporosis isoxazoline isoxazole prepn; osteoarthritis isoxazoline isoxazole prepn; tumor metastasis isoxazoline isoxazole prepn; diabetic retinopathy isoxazoline isoxazole prepn; antiinflammatory drug isoxazoline isoxazole prepn

IT Osteoarthritis

Osteoporosis

Psoriasis

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RL: BAC (Biological activity or effector, except adverse); BSU  
(Biological study, unclassified); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(preparation of novel isoxazoline and isoxazole fibrinogen receptor  
antagonists)

IT 170724-02-4P 185967-17-3P

RL: BAC (Biological activity or effector, except adverse); BSU  
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(Uses)

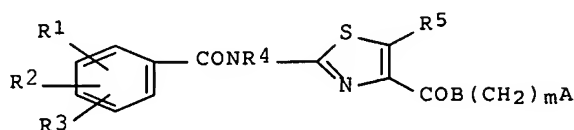
(preparation of novel isoxazoline and isoxazole fibrinogen receptor  
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RN 170724-02-4 HCAPLUS

CN Alanine, 3-[[[3-[4-(aminoiminomethyl)phenyl]-4,5-dihydro-5-  
isoxazolyl]acetyl]amino]-N-(4-iodophenyl)-, methyl ester (9CI) (CA INDEX  
NAME)

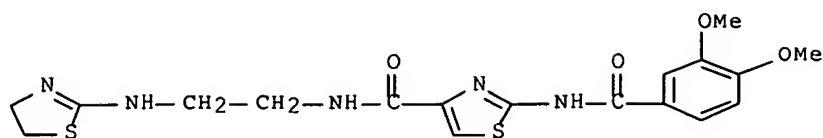
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WO 9636619	A1	19961121	WO 1996-JP1297	19960516 <--
W: AU, CA, CN, JP, KR, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2219747	A1	19961121	CA 1996-2219747	19960516 <--
AU 9657024	A	19961129	AU 1996-57024	19960516 <--
AU 699008	B2	19981119		
CN 1184471	A	19980610	CN 1996-194002	19960516 <--
CN 1063442	B	20010321		
EP 870765	A1	19981014	EP 1996-915167	19960516 <--
EP 870765	B1	20031119		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 3181919	B2	20010703	JP 1996-534703	19960516 <--
AT 254609	T	20031215	AT 1996-915167	19960516 <--
PT 870765	T	20040331	PT 1996-915167	19960516 <--
ES 2210366	T3	20040701	ES 1996-915167	19960516 <--
TW 445260	B	20010711	TW 1996-85105855	19960517 <--
US 5981557	A	19991109	US 1997-952106	19971118 <--
PRIORITY APPLN. INFO.:			JP 1995-142399	A 19950518 <--
			WO 1996-JP1297	W 19960516 <--
OTHER SOURCE(S):			MARPAT 126:59946	
GI				



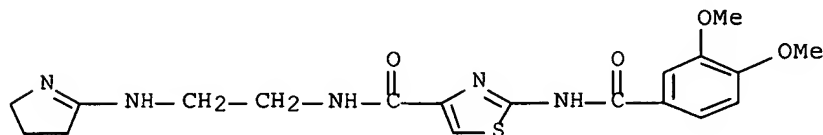
I

- AB The title compds. (I; R1, R2, R3 = H, OH, lower alkyl or alkoxy, etc.; R4 = H, lower alkyl; R5 = H, halo, lower alkyl; m = 0-4; A = substituted amino or imino, heterocycle, etc.; B = imino, O) are prepared I, having potent effects of promoting the movements of the digestive tracts, are useful as drugs for upper-abdomen discomfort, malevolence, vomiting, heart burn, appetite loss, stomach pain, feeling of abdominal inflation, chronic stomach inflammation, reflux esophagitis, and postgastrectomy syndrome. Thus, 2-[N-(4,5-dimethoxy-2-hydroxybenzoyl)amino]-4-(ethoxycarbonyl)-1,3-thiazole.ACOH (preparation given) was reacted with (Me2CHNHCH2)2 to give 69% I [R1 = 2-OH, R2 = 4-MeO, R3 = 5-MeO, R4 = R5 = H, m = 2, A = (Me2CH)2N, B = NH] (II). II at 1 mg/kg showed 213.3% movement coefficient when tested on dog i.v.
- IC ICM C07D277-56  
 ICS C07D417-12; A61K031-425; A61K031-44; A61K031-445; A61K031-495
- CC 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1, 63
- IT Pain  
 (Stomach; preparation of aminothiazole derivs. as ameliorating agents for



RN 185103-99-5 HCAPLUS

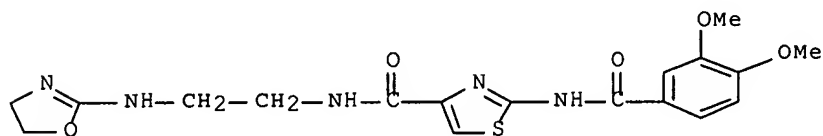
CN 4-Thiazolecarboxamide, N-[2-[(3,4-dihydro-2H-pyrrol-5-yl)amino]ethyl]-2-[(3,4-dimethoxybenzoyl)amino]-, monohydriodide (9CI) (CA INDEX NAME)



● HI

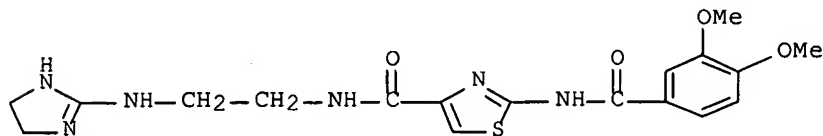
RN 185104-00-1 HCAPLUS

CN 4-Thiazolecarboxamide, N-[2-[(4,5-dihydro-2-oxazolyl)amino]ethyl]-2-[(3,4-dimethoxybenzoyl)amino]- (CA INDEX NAME)



RN 185104-01-2 HCAPLUS

CN 4-Thiazolecarboxamide, N-[2-[(4,5-dihydro-1H-imidazol-2-yl)amino]ethyl]-2-[(3,4-dimethoxybenzoyl)amino]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

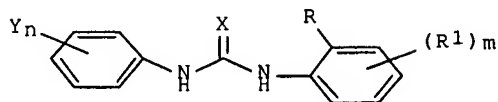
RN 185104-39-6 HCAPLUS

CN 4-Thiazolecarboxamide, 2-[(3,4-dimethoxybenzoyl)amino]-N-[2-(2-pyridinylamino)ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

CA 2432662	A1	19970821	CA 1996-2432662	19960821 <--
WO 9729743	A1	19970821	WO 1996-US13632	19960821 <--
W: AL, AM, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KG, KP, KR, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AZ, BY, KZ, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9669007	A	19970902	AU 1996-69007	19960821 <--
AU 725456	B2	20001012		
EP 896531	A1	19990217	EP 1996-929723	19960821 <--
R: AT, ES, GR, LU, SE, MC, PT, IE, SI, LT, LV, FI				
CN 1215990	A	19990505	CN 1996-180245	19960821 <--
JP 2000504722	T	20000418	JP 1997-529318	19960821 <--
NZ 316710	A	20000526	NZ 1996-316710	19960821 <--
HU 2000000467	A2	20000528	HU 2000-467	19960821 <--
HU 2000000467	A3	20000628		
BR 9612779	A	20001024	BR 1996-12779	19960821 <--
CN 1539816	A	20041027	CN 2004-10032423	19960821 <--
US 6005008	A	19991221	US 1997-894291	19970815 <--
US 6211373	B1	20010403	US 1998-111663	19980708 <--
NO 9803737	A	19981014	NO 1998-3737	19980814 <--
US 6180675	B1	20010130	US 1999-240354	19990129 <--
PRIORITY APPLN. INFO.:			US 1995-390260	A2 19950217 <--
			WO 1996-US2260	W 19960216 <--
			US 1996-641990	A3 19960320 <--
			CA 1996-2245927	A3 19960821 <--
			US 1996-701299	A3 19960821 <--
			WO 1996-US13632	W 19960821 <--

OTHER SOURCE(S): MARPAT 125:275430

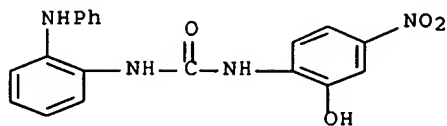
GI



AB The title compds. [I; X = O, S; R = any functional moiety having an ionizable H and a pKa of  $\leq 10$ ; R1, Y = H, halo, NO<sub>2</sub>, cyano, C1-10 (halo)alkyl, C2-10 alkenyl, C1-10 (halo)alkoxy, N3, HO, C1-4 hydroxyalkyl, aryl, aryl-C1-4 alkyl, aryloxy, aryl-C1-4 alkoxy, heteroaryl, heteroarylalkyl, heterocyclyl, heterocyclyl-C1-4 alkyl, heterocyclyl-C1-4 alkoxy, aryl-C2-10 alkenyl, heteroaryl-C2-10 alkenyl, (un)substituted NH<sub>2</sub>, carbamoyl, or SO<sub>3</sub>H, etc.; m, n = 1-3], which are useful for the treatment of disease states mediated by the chemokine, interleukin-8 (IL-8) (no data), are prepared. The chemokine-mediated disease is selected from psoriasis or atopic dermatitis, asthma, chronic obstructive pulmonary disease, adult respiratory distress syndrome, arthritis, inflammatory bowel disease, Crohn's disease, ulcerative colitis, septic shock, endotoxic shock, gram neg. sepsis, toxic shock syndrome, stroke, cardiac and renal reperfusion injury, glomerulo-nephritis, thrombosis, Alzheimer's disease, graft vs. host reaction, and allograft rejections. Thus, 1.19 mmol Me 4-amino-3-hydroxybenzoate was added to a solution of 1.19 mmol Ph isocyanate in toluene and the resulting mixture was stirred at .apprx.80° for 24-48 h to give 90% N-[2-hydroxy-4- (methoxycarbonyl)phenyl]-N'-phenylurea.

IC ICM A61K031-17

CN Urea, N-(2-hydroxy-4-nitrophenyl)-N'-[2-(phenylamino)phenyl]- (CA INDEX NAME)



L163 ANSWER 36 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:118765 HCAPLUS Full-text

DOCUMENT NUMBER: 124:220177

TITLE: Synthesis and pharmacological properties of 2,4-disubstituted 5-amino-6-pyrimidinecarboxylic acid derivatives. Part III

AUTHOR(S): Jaszold-Howorko, Ryszard; Machon, Zdzislaw; Wilimowski, Marian; Wojewodzki, Wieslaw; Barczynska, Jadwiga; Kedzierska, Lidia; Orzechowska-Juzwenko, Krystyna; Dus, Ewa; Dziewiszek, Wojciech; et al.

CORPORATE SOURCE: Department of Organic Chemistry, Medical Academy, Wroclaw, 50-137, Pol.

SOURCE: Polish Journal of Pharmacology (1995), 47(5), 435-40

CODEN: PJPAE3; ISSN: 1230-6002

PUBLISHER: Polish Academy of Sciences, Institute of Pharmacology

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 2,4-Disubstituted 5-amino-6-pyrimidinecarboxylic acids were synthesized and evaluated for their pharmacol. activity. Some of the compds. showed antiaggressive effect, while the piperidine-substituted compound exerted analgesic activity.

CC 1-11 (Pharmacology)  
Section cross-reference(s): 28

ST analgesic aminopyrimidinecarboxylate prepn structure; anxiolytic aminopyrimidinecarboxylate prepn structure; aminopyrimidinecarboxylate pharmacol prepn structure; pyrimidinecarboxylate amine pharmacol prepn structure

IT Analgesics  
Anxiolytics

(preparation and pharmacol. of disubstituted aminopyrimidinecarboxylic acids)

IT Molecular structure-biological activity relationship  
(analgesic, preparation and pharmacol. of disubstituted aminopyrimidinecarboxylic acids)

IT 59662-97-4P 174805-11-9P 174805-12-0P  
174805-13-1P 174805-14-2P 174805-15-3P  
174805-16-4P 174805-17-5P 174805-18-6P

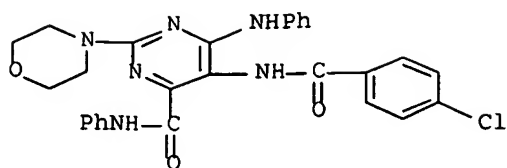
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and pharmacol. of aminopyrimidinecarboxylic acids)

IT 146073-96-3

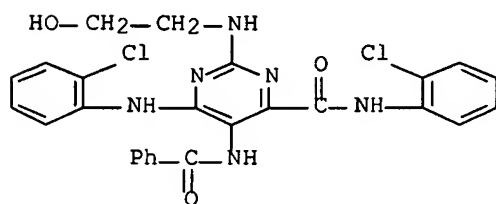
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation and pharmacol. of aminopyrimidinecarboxylic acids)



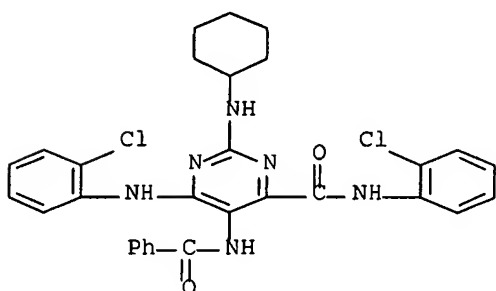
RN 174805-14-2 HCAPLUS

CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-N-(2-chlorophenyl)-6-[(2-chlorophenyl)amino]-2-[(2-hydroxyethyl)amino]- (CA INDEX NAME)



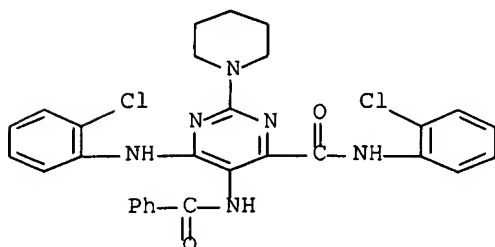
RN 174805-15-3 HCAPLUS

CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-N-(2-chlorophenyl)-6-[(2-chlorophenyl)amino]-2-(cyclohexylamino)- (CA INDEX NAME)



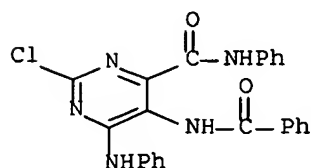
RN 174805-16-4 HCAPLUS

CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-N-(2-chlorophenyl)-6-[(2-chlorophenyl)amino]-2-(1-piperidinyl)- (CA INDEX NAME)



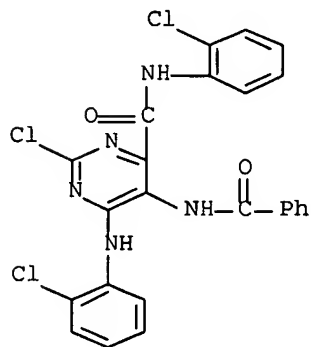
RN 59662-92-9 HCAPLUS

CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-2-chloro-N-phenyl-6-(phenylamino)- (CA INDEX NAME)



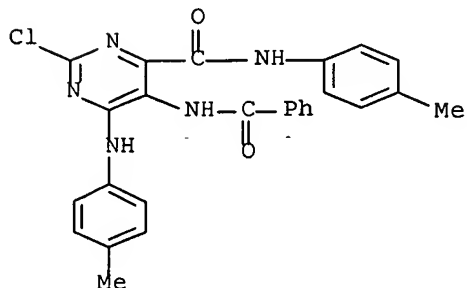
RN 146073-99-6 HCAPLUS

CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-2-chloro-N-(2-chlorophenyl)-6-[(2-chlorophenyl)amino]- (CA INDEX NAME)



RN 146074-06-8 HCAPLUS

CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-2-chloro-N-(4-methylphenyl)-6-[(4-methylphenyl)amino]- (CA INDEX NAME)



L163 ANSWER 37 OF 39 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:580492 HCAPLUS Full-text

DOCUMENT NUMBER: 122:314570

TITLE: Preparation of heterocyclylnaphthalene derivatives as serotonin 5-HT1 agonists and antagonists.

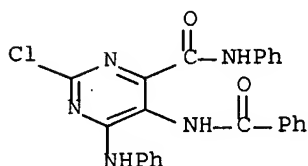
INVENTOR(S): Chenard, Bertrand L.; Macor, John E.; Segelstein,



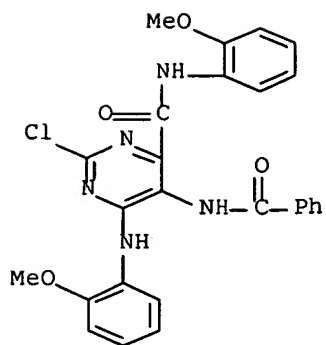
alkylaryl, aryl; R4, R5 = Q4, Q5, H, CF3, alkyl, alkylaryl, etc.; R6-R14 = H, halo, CF3, CN, NO2, aryl, alkylaryl, alkyl, alkenyl, alkynyl, OR20, COR20, NR20R21, etc.; adjacent pairs of R6-R14 = atoms to form 5-7 membered rings; R20, R21 = H, alkyl, aryl, alkylaryl; R20R21 = atoms to form 4-7 membered rings; A, B, D, E, F, L = C, N; G, I, J, K = C, N, O, S, C=O; X = O, S; a = 0-2; b, c = 0-6; dotted line = optional double bond; with provisos], were prepared. These compds. are useful psychotherapeutics and are potent serotonin (5-HT1) agonists and antagonists and may be used in the treatment of depression, anxiety, eating disorders, obesity, drug abuse, cluster headache, migraine, pain and chronic paroxysmal hemicrania and headache associated with vascular disorders, and other disorders arising from deficient serotonergic neurotransmission. The compds. can also be used as centrally acting antihypertensives and vasodilators. Thus, 7-amino- $\alpha$ -tetralone was stirred with PhCOCl/Et3N in THF to give 85% 7-benzamido- $\alpha$ -tetralone. This in THF at -78° was treated with N-methylpiperazine and TiCl4 to give 83% 7-benzamido-1-(4-methyl-1-piperazinyl)-3,4-dihydronaphthalene. The latter was refluxed with Pd/C in xylene to give title compound 7-benzamido-1-(4-methyl-1-piperazinyl)naphthalene and 7-benzamido-1-(4-methyl-1-piperazinyl)-1,2,3,4-tetrahydronaphthalene. I showed IC50 <0.60 nM for 5-HT1A and/or 5-HT1D affinity.

- IC ICM C07D295-135  
ICS C07D295-096; C07D295-033; C07D295-155; C07D207-09; C07D213-74;  
C07D211-26; C07D213-57; C07D471-04; C07D235-04; C07D401-12;  
A61K031-495; A61K031-445; A61K031-40
- CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1
- IT Analgesics  
Antidepressants  
Antihypertensives  
Antiobesity agents  
Anxiolytics  
(preparation of heterocyclylnaphthalene derivs. as serotonin 5-HT1 agonists and antagonists)
- IT Drug dependence  
Headache  
(treatment; preparation of heterocyclylnaphthalene derivs. as serotonin 5-HT1 agonists and antagonists)
- IT Headache  
(cluster, treatment; preparation of heterocyclylnaphthalene derivs. as serotonin 5-HT1 agonists and antagonists)
- IT Headache  
(migraine, treatment; preparation of heterocyclylnaphthalene derivs. as serotonin 5-HT1 agonists and antagonists)
- IT 163464-92-4P 163464-93-5P 163464-94-6P 163464-95-7P 163464-96-8P  
163464-97-9P 163464-98-0P 163464-99-1P 163465-00-7P 163465-01-8P  
163465-02-9P 163465-03-0P 163465-04-1P 163465-05-2P 163465-06-3P  
163465-07-4P 163465-08-5P 163465-09-6P 163465-10-9P 163465-11-0P  
163465-12-1P 163465-13-2P 163465-14-3P 163465-15-4P 163465-16-5P  
163465-17-6P 163465-18-7P 163465-19-8P 163465-20-1P  
163465-21-2P 163465-22-3P 163465-23-4P 163465-24-5P 163465-25-6P  
163465-26-7P 163465-28-9P 163465-29-0P 163465-30-3P 163465-31-4P  
163465-32-5P 163465-33-6P 163465-34-7P 163465-35-8P 163465-36-9P  
163465-37-0P 163465-38-1P 163465-39-2P 163465-40-5P 163465-41-6P  
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163465-72-3P 163465-73-4P 163465-74-5P 163465-75-6P 163498-49-5P

- AB 2,4-Disubstituted 5-amino-6-pyrimidinecarboxylic acid derivs. (I; R = H or Cl; R1 = alkyl- or arylamino) were synthesized and evaluated for their pharmacol. activity on the central nervous system. Some compds. had an antiaggressive effect, others displayed antiserotonin activity, while 1 compound exerted antireserpine action. Structure-activity relations are discussed.
- CC 1-3 (Pharmacology)  
Section cross-reference(s): 28
- IT Analgesics  
Anticonvulsants and Antiepileptics  
Nervous system agents  
(aminopyrimidinecarboxylate derivs. as)
- IT 59662-91-8P 59662-92-9P 59662-94-1P 146073-95-2P  
146073-96-3P 146073-97-4P 146073-98-5P  
146073-99-6P 146074-00-2P 146074-01-3P  
146074-02-4P 146074-03-5P 146074-04-6P  
146074-05-7P 146074-06-8P 146074-07-9P  
146074-08-0DP, derivs.  
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)  
(preparation and pharmacol. of, structure in relation to)
- IT 59662-92-9P 59662-94-1P 146073-96-3P  
146073-97-4P 146073-98-5P 146073-99-6P  
146074-00-2P 146074-01-3P 146074-02-4P  
146074-03-5P 146074-04-6P 146074-05-7P  
146074-06-8P 146074-07-9P  
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)  
(preparation and pharmacol. of, structure in relation to)
- RN 59662-92-9 HCAPLUS
- CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-2-chloro-N-phenyl-6-(phenylamino)- (CA INDEX NAME)

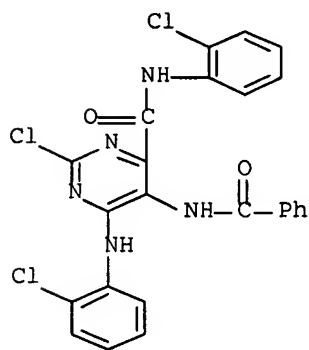


- RN 59662-94-1 HCAPLUS
- CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-2-chloro-N-(4-chlorophenyl)-6-[(4-chlorophenyl)amino]- (CA INDEX NAME)



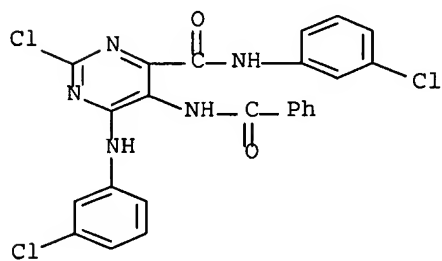
RN 146073-99-6 HCAPLUS

CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-2-chloro-N-(2-chlorophenyl)-6-[(2-chlorophenyl)amino]- (CA INDEX NAME)



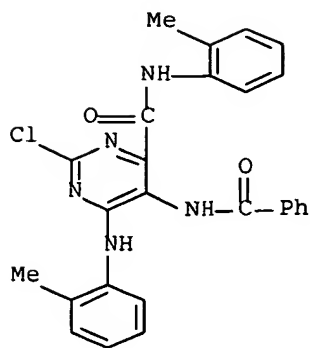
RN 146074-00-2 HCAPLUS

CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-2-chloro-N-(3-chlorophenyl)-6-[(3-chlorophenyl)amino]- (CA INDEX NAME)



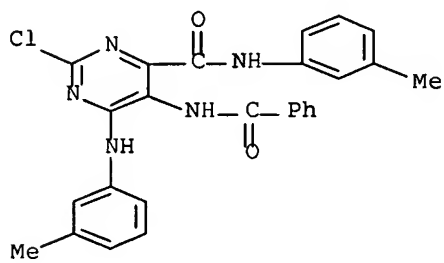
RN 146074-01-3 HCAPLUS

CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-2-chloro-N-(2,4-dichlorophenyl)-6-[(2,4-dichlorophenyl)amino]- (CA INDEX NAME)



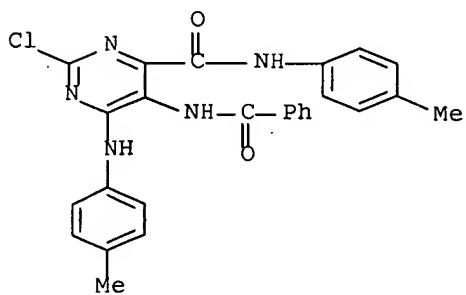
RN 146074-05-7 HCAPLUS

CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-2-chloro-N-(3-methylphenyl)-6-[(3-methylphenyl)amino]- (CA INDEX NAME)



RN 146074-06-8 HCAPLUS

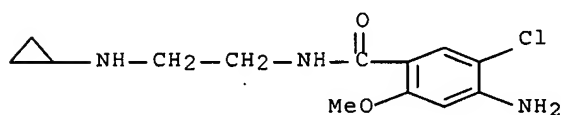
CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-2-chloro-N-(4-methylphenyl)-6-[(4-methylphenyl)amino]- (CA INDEX NAME)



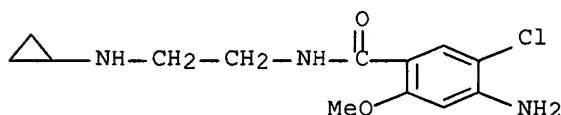
RN 146074-07-9 HCAPLUS

CN 4-Pyrimidinecarboxamide, 5-(benzoylamino)-2-chloro-N-(5-methyl-2-pyridinyl)-6-[(5-methyl-2-pyridinyl)amino]- (CA INDEX NAME)

CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 Section cross-reference(s): 1  
 IT Digestion, biological  
 Headache  
 Nausea  
 (treatment of, by cycloalkylaminoethylbenzamides)  
 IT 126105-15-5P 126105-16-6P 126105-17-7P  
 126105-18-8P 126105-19-9P 126105-20-2P  
 126132-64-7P  
 RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); BIOL  
 (Biological study); PREP (Preparation)  
 (preparation of, as drug)  
 IT 126105-15-5P 126105-16-6P 126105-17-7P  
 126105-18-8P 126105-19-9P 126105-20-2P  
 RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); BIOL  
 (Biological study); PREP (Preparation)  
 (preparation of, as drug)  
 RN 126105-15-5 HCAPLUS  
 CN Benzamide, 4-amino-5-chloro-N-[2-(cyclopropylamino)ethyl]-2-methoxy- (CA  
 INDEX NAME)

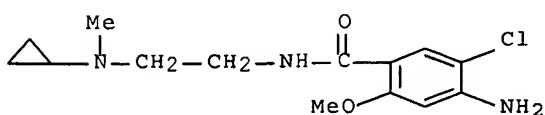


RN 126105-16-6 HCAPLUS  
 CN Benzamide, 4-amino-5-chloro-N-[2-(cyclopropylamino)ethyl]-2-methoxy-,  
 hydrochloride (9CI) (CA INDEX NAME)



●x HCl

RN 126105-17-7 HCAPLUS  
 CN Benzamide, 4-amino-5-chloro-N-[2-(cyclopropylmethylamino)ethyl]-2-methoxy-  
 (CA INDEX NAME)



RN 126105-18-8 HCAPLUS

## STRUCTURE + DRUG SCREENING

=&gt; d que nos 1139

L42 SCR 1839 AND 1993  
 L50 STR  
 L52 SCR 392 OR 391  
 L73 SCR 1952  
 L81 57965 SEA FILE=REGISTRY SSS FUL (L50) AND L42 AND L52 AND L73  
 L84 53736 SEA FILE=REGISTRY SSS FUL (L50) AND L42 AND L52 NOT L73  
 L85 111701 SEA FILE=REGISTRY ABB=ON (L81 OR L84)  
 L87 STR  
 L88 STR  
 L89 STR  
 L90 STR  
 L93 8317 SEA FILE=REGISTRY SUB=L85 SSS FUL (L50 NOT (L87 OR L88 OR L89 OR L90))  
 L94 1407 SEA FILE=HCAPLUS ABB=ON L93  
 L130 912 SEA FILE=HCAPLUS ABB=ON L94 AND (PY<2001 OR AY<2001 OR PRY<2001)  
 L138 56795 SEA FILE=HCAPLUS ABB=ON SCREENING/CW  
 L139 4 SEA FILE=HCAPLUS ABB=ON L130 AND L138

=&gt; s 1139 not 196,1163

L164 3 L139 NOT (L96 OR L163)

=&gt; d ibib abs hitind hitstr 1164 1-3

L164 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:20322 HCAPLUS Full-text

DOCUMENT NUMBER: 140:87658

TITLE: Peptidomimetic modulators of cell adhesion

INVENTOR(S): Gour, Barbara J.; Blaschuk, Orest W.; Ali, Anmar; Ni, Feng; Chen, Zhigang; Michaud, Stephanie Denise; Wang, Shaomeng; Hu, Zengjian

PATENT ASSIGNEE(S): Can.

 SOURCE: U.S. Pat. Appl. Publ., 280 pp., Cont.-in-part of U.S. Ser. No. 6,982.  
 CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 15

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004006011	A1	20040108	US 2003-425557	20030428 <--
US 6031072	A	20000229	US 1997-893534	19970711 <--
US 6326352	B1	20011204	US 2000-507102	20000217 <--
US 2002168761	A1	20021114	US 2001-769145	20010124 <--
US 2002151475	A1	20021017	US 2001-6982	20011204 <--
US 6914044	B2	20050705		
PRIORITY APPLN. INFO.:			US 1996-21612P	P 19960712 <--
			US 1997-893534	A1 19970711 <--
			US 2000-491078	B2 20000124 <--
			US 2000-507102	A1 20000217 <--
			US 2001-769145	B2 20010124
			US 2001-6982	A2 20011204

OTHER SOURCE(S): MARPAT 140:87658

5341-00-4, 1,4-Naphthalenedione, 2-[3-(decahydro-2-naphthalenyl)propyl]-3-hydroxy- 5415-88-3, 1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-8-(4-phenylbutoxy)- 5421-95-4, Urea, (3-phenyl-1,2,4-oxadiazol-5-yl)- 5426-87-9, Benzamide, N-[(2,3,6,7-tetrahydro-1,3-dimethyl-2,6-dioxo-1H-purin-8-yl)methyl]- 5429-46-9, Benzamide, N-[2-(2,3,6,7-tetrahydro-1,3-dimethyl-2,6-dioxo-1H-purin-8-yl)ethyl]- 5446-36-6, 1H-Purin-6-amine, N-(4-methylphenyl)- 5454-50-2, Ethanone, 1-phenyl-2-(1H-purin-6-ylthio)- 5454-52-4, 1H-Purine, 6-[(2-phenoxyethyl)thio]- 5508-58-7, 2(3H)-Furanone, 3-[2-[(1R,4aS,5R,6R,8aS)-decahydro-6-hydroxy-5-(hydroxymethyl)-5,8a-dimethyl-2-methylene-1-naphthalenyl]ethylidene]dihydro-4-hydroxy-, (3E,4S)- 5534-95-2 5786-82-3, L-Glutamic acid, N-[4-[[2-(2-amino-1,5,6,7-tetrahydro-4-hydroxy-6-pteridiny]ethyl)amino]benzoyl]- 5800-34-0, Pentanoic acid, 5-[[[(1S)-2-[(4-nitrophenyl)amino]-2-oxo-1-(phenylmethyl)ethyl]amino]-5-oxo-6286-57-3, 5(4H)-Isoxazolone, 4-(1,3-benzodioxol-5-ylmethylene)-3-phenyl- 6295-27-8, 7H-1,2,3-Triazolo[4,5-d]pyrimidin-7-one, 5-amino-2,6-dihydro-2-phenyl- 6300-80-7, Benzaldehyde, 4-(dimethylamino)-, 7H-purin-6-ylhydrazone 6320-71-4, 1,4-Naphthalenedione, 2-(4-cyclohexylbutyl)-3-hydroxy- 6322-09-4, 2(1H)-Quinoxalinone, 3-[2-(2-chlorophenyl)ethenyl]-7-methyl- 6323-88-2, 2(1H)-Quinoxalinone, 3-[2-(3-nitrophenyl)ethenyl]- 6323-89-3, 2(1H)-Quinoxalinone, 3-(2-phenylethenyl)- 6331-03-9, Benzaldehyde, 4-nitro-, 7H-purin-6-ylhydrazone 6338-84-7, 1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-8-(2-phenylethyl)- 6340-76-7, 2,4-Pyrimidinediamine, 6-chloro-N4-(3-methylphenyl)- 6633-66-5, 2,4,6-Pyrimidinetriamine, N4-(4-bromophenyl)- 6807-82-5, L-Glutamic acid, N-[4-[[[(2-amino-1,4-dihydro-4-oxo-6-pteridiny]methyl)amino]benzoyl]-L- $\alpha$ -glutamyl]- 6962-62-5, 2-Propen-1-one, 3-(1,3-benzodioxol-5-yl)-1-(2,4-dihydroxyphenyl)- 6975-34-4, 1H-Purine, 6-[(3-phenyl-2-propenyl)thio]- 7781-29-5, 2,4-Pyrimidinediamine, 6-methyl-N4-phenyl- 10320-97-5, 1,2,3,4-Thiatriazol-5-amine, N-1-naphthalenyl- 13184-14-0, L-Lysine, L-lysyl-L-lysyl- 13351-10-5, 2-Propen-1-one, 1-(2,4-dihydroxyphenyl)-3-(4-methoxyphenyl)- 13745-20-5, 2-Propen-1-one, 1-(2,4-dihydroxyphenyl)-3-(4-hydroxyphenyl)- 15013-60-2, Cholest-4-ene-3,6-diol, (3 $\beta$ ,6 $\alpha$ )- 15970-42-0, 1H-Imidazole-1,2-diamine, 4-(4-chlorophenyl)- 16856-21-6, L-Tryptophan, N-[N-[(phenylmethoxy)carbonyl]-L-phenylalanyl]-, methyl ester 16879-84-8, L-Threonine, N-[(phenylmethoxy)carbonyl]-, (4-nitrophenyl)methyl ester 17357-75-4, 1H-1,2,4-Triazole, 3-[[[(4-methoxyphenyl)methyl]thio]- 17430-65-8, L-Tryptophan, N-[(phenylmethoxy)carbonyl]-L-valyl-, methyl ester 17496-31-0, 1H-Imidazole, 4-[[[(phenylmethyl)thio]methyl]- 18100-11-3, 1,4-Naphthalenedione, 2-(3-cyclohexylbutyl)-3-hydroxy- 18100-12-4, 1,4-Naphthalenedione, 2-[3-(4-chlorophenyl)propyl]-3-hydroxy- 18211-37-5, 1,4-Naphthalenedione, 2-hydroxy-3-[3-(4-methylphenyl)propyl]- 19312-13-1, 2-Propen-1-one, 1-(2,5-dihydroxyphenyl)-3-phenyl- 19484-75-4D, 2H-1-Benzopyran-2-one, 3,4-dihydro-7-hydroxy-4-methyl-, furanoside derivative 19889-31-7, 1H-Imidazole-4-propanamide,  $\alpha$ -amino-N-2-naphthalenyl- 20621-49-2, 2-Propen-1-one, 1-(2,6-dihydroxy-4-methoxyphenyl)-3-(4-methoxyphenyl)- 21108-76-9, Imidazo[2,1-b]thiazol-3(2H)-one, 5,6-dihydro-2-(3-phenyl-2-propenylidene)- 21658-45-7, Glycine, L-arginyl-L-prolyl-L-prolyl- 23567-67-1, Phenol, 4-(1,2,3,4-thiatriazol-5-ylamino)- 23815-88-5, 1-6-Bradykinin 24205-32-1, L-Glutamic acid, N-[4-[[[(2,4-diamino-5-methyl-6-quinazolinyl)methyl]amino]benzoyl]-, diethylester 24386-39-8, Urea, N-1-naphthalenyl-N'-2-pyrimidinyl- 24829-12-7, Phenol, 2-[(1H-1,2,4-triazol-3-ylimino)methyl]- 26962-50-5, 2-Propen-1-one, 1-(2,4-dihydroxyphenyl)-3-(2-hydroxyphenyl)- 27069-81-4, L-Glutamic acid, N-[4-[[[(2-amino-1,4-dihydro-4-oxo-6-quinazolinyl)methyl]amino]benzoyl]

yl]-, 5-butyl ester 67368-29-0, L-Alanine, L-methionyl-L-arginyl-L-phenylalanyl- 67655-19-0, Phenol, 2,2'-[(2-hydroxy-1,3-propanediyl)bis(oxy)]bis- 67836-16-2, Acetamide, 2-(2,4-dichlorophenoxy)-N-1H-1,2,4-triazol-3-yl- 68047-41-6, 1,3,4-Oxadiazole, 2-(3-bromophenyl)-5-(2-naphthalenyl)- 68215-68-9, Phenol, 2-[4-amino-6-[(4-chlorophenyl)amino]-1,3,5-triazin-2-yl]-4-chloro-68682-02-0, 4H-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-8-(3-methyl-2-butenyl)- 68838-40-4, 1H-1,2,4-Triazole, 3-methyl-5-[(phenylmethyl)thio]- 69097-98-9, 4H-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)- 69193-20-0, 4-Pyrimidinamine, 5-bromo-N-phenyl- 69480-15-5, 3H-1,2,4-Triazole-3-thione, 5-[4-(1,1-dimethylethyl)phenyl]-1,2-dihydro- 70280-72-7, L-Glutamic acid, N-[4-[(2,4-diamino-6-pteridinyl)methyl](phenylmethyl)amino]benzoyl]-, diethyl ester 70280-75-0, L-Glutamic acid, N-[4-[(2,4-diamino-6-pteridinyl)methyl]ethylamino]benzoyl]-, diethyl ester 70539-54-7, L-Glutamic acid, N-[3,5-dichloro-4-[(2,4-diamino-6-pteridinyl)methyl]ethylamino]benzoyl]-, diethyl ester 70968-04-6, L-Leucinamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-alanyl-L-prolyl-N-(4-nitrophenyl)- 71047-38-6, 1H-Imidazole, 1-(3,7-dimethyl-2,6-octadienyl)- 71074-46-9, Glycine, N-[N-[4-[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]-L-γ-glutamyl]- 71074-48-1, L-Aspartic acid, N-[4-[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]-L-α-glutamyl]- 71074-49-2, L-Glutamic acid, N-[4-[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]-L-α-glutamyl]- 71707-02-3, L-Glutamic acid, N-[N-[4-[(2,4-diamino-6-pteridinyl)methyl]amino]benzoyl]-L-γ-glutamyl]- 72630-15-0, Glutamic acid, N-[4-[[2-(2-amino-1,4,5,6,7,8-hexahydro-5-methyl-4-oxo-6-pteridinyl)ethyl]amino]benzoyl]- 72682-77-0, L-Isoleucinamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-alanyl-L-prolyl-N-(4-nitrophenyl)- 72704-76-8, 2-Propen-1-one, 3-(3,4-dihydroxyphenyl)-1-phenyl- 73554-90-2, L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-L-seryl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)- 73572-58-4, L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-L-leucyl-L-phenylalanyl-L-leucyl- 74039-67-1, 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(3-phenyl-2-propenyl)- 74405-42-8, Adenosine, N-benzoyl-5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-, 3'-(hydrogen butanedioate) 74405-44-0, Cytidine, N-benzoyl-5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-deoxy-, 3'-(hydrogen butanedioate) 74853-69-3, L-Leucine, N2-acetyl-L-arginyl-L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- 75651-68-2, L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-phenylalanyl-L-prolyl-N-(4-nitrophenyl)- 75960-43-9, 1H-Imidazole-4-hexanoic acid, 5-(chloromethyl)-2,3-dihydro-ε,2-dioxo-, ethyl ester 76172-68-4, 1-Propanone, 3-(4-methoxyphenyl)-1-(2,4,6-trihydroxyphenyl)- 80032-99-1, 1H-1,2,4-Triazole, 3,3'-[1,4-butanediylbis(thio)]bis- 80360-08-3, L-Glutamic acid, N-[4-[(2,4-diaminopyrido[2,3-d]pyrimidin-6-yl)methyl]amino]benzoyl]-, diethylester 81066-61-7, 2-Pyridinamine, 3-[[4-(1,1-dimethylethyl)phenyl]methoxy]- 81587-37-3, 3-Pyridinethiol, 2-[(2,6-diamino-4-pyrimidinyl)amino]-6-methyl- 82628-82-8, 1-Propanone, 3-(4-nitrophenyl)-1-(2,4,6-trihydroxyphenyl)- 82855-85-4, L-Glutamic acid, N-[4-[(2-amino-1,4,5,6,7,8-hexahydro-4-oxopyrido[3,2-d]pyrimidin-6-yl)methyl]amino]benzoyl]-, diethyl ester 85122-85-6, 1H-Isoindole-1,3(2H)-dione, 2,2'-[1,3-propanediylbis(4,1-piperidinediylmethylene)]bis- 86669-33-2, L-Glutamic acid, N-[4-[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]-, bis(1,1-dimethylethyl) ester 90259-60-2, Benzamide, 2-amino-N-[3-(1H-imidazol-1-yl)propyl]- 90259-61-3, Benzamide, 2-[[4-(4-chlorophenyl)sulfonyl]amino]-N-[3-(1H-imidazol-1-yl)propyl]- 92899-39-3, Glycine, L-valylglycyl-L-valyl-L-alanyl-L-prolyl- 92954-99-9, Glycine,



[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]-155373-59-4, 4H-1-Benzopyran-4-one, 3-[[4-(1H-tetrazol-5-yl)phenyl]methyl]-155373-72-1, 4H-1-Benzopyran-4-one, 2-phenyl-7-[4-(1H-tetrazol-5-yl)butoxy]-160347-57-9D, 2(1H)-Pyrimidinone, 5-(4-pentylphenyl)-, derivs. 185503-97-3, L-Lysine, N6-[[4-[[4-(dimethylamino)phenyl]azolphenyl]sulfonyl]-N2-[(9H-fluoren-9-ylmethoxy)carbonyl]-188966-22-5D, Phenol, 2-(2H-benzotriazol-2-yl)-4-(1,1-dimethylhexyl)-, derivs. 191411-47-9, 1H-Imidazole-5-methanol, 1-methyl-2-[(phenylmethyl)thio]-194424-08-3, Glutamic acid, N-[4-[[3-(2-thienyl)-2-quinoxaliny]amino]benzoyl]-, dipropyl ester 195140-70-6, 1H-Imidazole, 1-[2-(phenylmethoxy)ethyl]-196600-87-0, Tyrosine, N-[(phenylmethoxy)carbonyl]norvalylglycyl-, methyl ester 197456-56-7, 1,4-Naphthalenedione, 2-[4-(decahydro-2-naphthalenyl)butyl]-3-hydroxy-198488-04-9, Urea, N,N'-(3,3'-dimethyl[1,1'-biphenyl]-4,4'-diyl)bis[N'-(2-methylphenyl)-198632-08-5, L-Proline, glycyl-L-arginylglycyl-L- $\alpha$ -glutamyl-L-threonyl-199929-21-0, 1,4-Naphthalenedione, 2-hydroxy-3-[8-(4-methylphenoxy)octyl]-200058-34-0, 1,4-Naphthalenedione, 2-(3-[1,1'-bicyclohexyl]-4-ylpropyl)-3-hydroxy-200061-22-9, Phenol, 4,4'-(1-methylethylidene)bis-, bis(3,5-dinitrobenzoate) 200431-98-7, 3-Pyridinemethanamine, N-1H-1,2,4-triazol-3-yl-200505-51-7, Decanedioic acid, bis[[4-(ethoxy-3-methoxyphenyl)methylene]hydrazide] 200706-30-5, 4H-1,2,4-Triazol-4-amine, N-[(2,3-dihydro-1H-inden-5-yl)methylene]-200706-45-2, 4-Imidazolidinone, 5-[(2,3-dihydro-1H-inden-5-yl)methylene]-2-thioxo-201997-13-9, 1,3-Benzenediol, 4-[[[2-hydroxy-2-(4-nitrophenyl)ethyl]imino]methyl]-202118-27-2, 1H-1,2,4-Triazol-3-amine, N-[(2-iodophenyl)methylene]-202118-28-3, 1H-1,2,4-Triazol-3-amine, N-[(2-chlorophenyl)methylene]-202332-09-0, 1,4-Benzenediol, 2-(6-methylheptyl)-202528-15-2, Cyclo(L-alanyl-L-histidyl-L-alanyl-L-valyl-L- $\alpha$ -aspartyl-L-isoleucyl) 206360-24-9, 4H-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-(4-hydroxyphenyl)-3-(3-methyl-2-butenyl)-210709-22-1, L-Alanine, N2-benzoyl-L-arginyl-L-phenylalanyl-215434-58-5, 1-Piperazinecarbothioamide, N-3-pyridinyl-4-[4-(trifluoromethyl)-2-pyrimidinyl]-215655-36-0, Benzoic acid, 2-[[[2-[[4-(trifluoromethyl)-2-pyrimidinyl]amino]ethyl]amino]carbonyl]-215657-86-6, 2-Pyrrolidinone, 1-[2-hydroxy-3-[4-[4-(trifluoromethyl)-2-pyrimidinyl]-1-piperazinyl]propyl]-

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(peptidomimetic modulators of cadherin-mediated cell adhesion for therapeutic use in relation to three-dimensional structure)

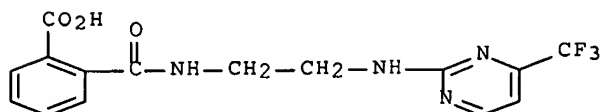
IT 215655-36-0, Benzoic acid, 2-[[[2-[[4-(trifluoromethyl)-2-pyrimidinyl]amino]ethyl]amino]carbonyl]-

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(peptidomimetic modulators of cadherin-mediated cell adhesion for therapeutic use in relation to three-dimensional structure)

RN 215655-36-0 HCAPLUS

CN Benzoic acid, 2-[[[2-[[4-(trifluoromethyl)-2-pyrimidinyl]amino]ethyl]amino]carbonyl]- (CA INDEX NAME)



Ovary, neoplasm  
 Peptidomimetics  
 Protein sequences  
 QSAR (quantitative structure-activity relationship)  
 Steric effects  
 Transplant and Transplantation  
 Wound healing  
 Wound healing promoters  
 (peptidomimetic modulators of cadherin-mediated cell adhesion for  
 therapeutic use in relation to three-dimensional structure)

IT 57-88-5D, Cholest-5-en-3-ol (3 $\beta$ )-, glycoside derivs. 135-16-0,  
 L-Glutamic acid, N-[4-[[2-amino-1,4,5,6,7,8-hexahydro-4-oxo-6-  
 pteridiny]methyl]amino]benzoyl]- 487-49-0, Ethanone,  
 1-(2,4-dihydroxyphenyl)-2-(4-methoxyphenyl)- 548-73-2,  
 2H-Benzimidazol-2-one, 1-[1-[4-(4-fluorophenyl)-4-oxobutyl]-1,2,3,6-  
 tetrahydro-4-pyridinyl]-1,3-dihydro- 570-88-7, Cholest-4-ene-3,6-diol,  
 (3 $\beta$ ,6 $\beta$ )- 1210-66-8, 1H-Purin-6-amine, N-phenyl- 1482-74-2,  
 2-Propen-1-one, 3-phenyl-1-(2,3,4-trihydroxyphenyl)- 1699-40-7,  
 Benzeneacetamide, 4-methoxy-N-[2-[3-methoxy-4-(phenylmethoxy)phenyl]ethyl]-  
 3-(phenylmethoxy)- 1776-30-3, 2-Propen-1-one, 1-(2,4-dihydroxyphenyl)-3-  
 phenyl- 2486-02-4, Benzoic acid, 3,4,5-trihydroxy-, 3-methylbutyl ester  
 2810-37-9, 1H-Isoindole-1,3(2H)-dione, 2-[5-(1H-benzotriazol-1-yl)propyl]-  
 2979-51-3, 1H-Imidazole, 1-(1-oxo-3-phenyl-2-propenyl)- 3242-68-0,  
 L-Glutamic acid, N-[4-[[2-[(2-amino-1,4-dihydro-4-oxo-5-  
 pyrimidinyl)amino]ethyl]amino]benzoyl]- 3257-73-6, 9H-Purin-6-amine,  
 9-[2,3,5-tris-O-(phenylmethyl)- $\beta$ -D-arabinofuranosyl]- 3561-56-6,  
 L-Asparagine, N2-[(phenylmethoxy)carbonyl]-, (4-nitrophenyl)methyl ester  
 3566-25-4, L-Glutamic acid, N-[4-[[2-(2-amino-1,4-dihydro-4-oxo-6-  
 pteridiny]ethyl]amino]benzoyl]- 3575-07-3, 1H-Benzimidazole,  
 2,2'-(1,2-ethanediyl)bis- 3922-47-2, 1H-1,2,4-Triazol-3-amine,  
 5-[(phenylmethyl)thio]- 4672-96-2, Benzeneacetamide,  
 3-methoxy-N-[2-[4-methoxy-3-(phenylmethoxy)phenyl]ethyl]-4-(phenylmethoxy)-  
 5226-71-1, Benzene, 1,1'-[1,10-decanediylbis(oxy)]bis[3-nitro-  
 5341-00-4, 1,4-Naphthalenedione, 2-[3-(decahydro-2-naphthalenyl)propyl]-3-  
 hydroxy- 5415-88-3, 1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-8-  
 (4-phenylbutoxy)- 5421-95-4, Urea, (3-phenyl-1,2,4-oxadiazol-5-yl)-  
 5426-87-9, Benzamide, N-[(2,3,6,7-tetrahydro-1,3-dimethyl-2,6-dioxo-1H-  
 purin-8-yl)methyl]- 5429-46-9, Benzamide, N-[2-(2,3,6,7-tetrahydro-1,3-  
 dimethyl-2,6-dioxo-1H-purin-8-yl)ethyl]- 5446-36-6, 1H-Purin-6-amine,  
 N-(4-methylphenyl)- 5454-50-2, Ethanone, 1-phenyl-2-(1H-purin-6-ylthio)-  
 5454-52-4, 1H-Purine, 6-[(2-phenoxyethyl)thio]- 5508-58-7,  
 2(3H)-Furanone, 3-[2-[(1R,4aS,5R,6R,8aS)-decahydro-6-hydroxy-5-  
 (hydroxymethyl)-5,8a-dimethyl-2-methylene-1-naphthalenyl]ethylidene]dihydr  
 o-4-hydroxy-, (3E,4S)- 5534-95-2 5786-82-3, L-Glutamic acid,  
 N-[4-[[2-(2-amino-1,5,6,7-tetrahydro-4-hydroxy-6-  
 pteridiny]ethyl]amino]benzoyl]- 5800-34-0, Pentanoic acid,  
 5-[[[(1S)-2-[(4-nitrophenyl)amino]-2-oxo-1-(phenylmethyl)ethyl]amino]-5-oxo-  
 6286-57-3, 5(4H)-Isoxazolone, 4-(1,3-benzodioxol-5-ylmethylene)-3-  
 phenyl- 6295-27-8, 7H-1,2,3-Triazolo[4,5-d]pyrimidin-7-one,  
 5-amino-2,6-dihydro-2-phenyl- 6300-80-7, Benzaldehyde,  
 4-(dimethylamino)-, 7H-purin-6-ylhydrazone 6320-71-4,  
 1,4-Naphthalenedione, 2-(4-cyclohexylbutyl)-3-hydroxy- 6322-09-4,  
 2(1H)-Quinoxalinone, 3-[2-(2-chlorophenyl)ethenyl]-7-methyl- 6323-88-2,  
 2(1H)-Quinoxalinone, 3-[2-(3-nitrophenyl)ethenyl]- 6323-89-3,  
 2(1H)-Quinoxalinone, 3-(2-phenylethenyl)- 6331-03-9, Benzaldehyde,  
 4-nitro-, 7H-purin-6-ylhydrazone 6338-84-7, 1H-Purine-2,6-dione,  
 3,7-dihydro-1,3,7-trimethyl-8-(2-phenylethyl)- 6340-76-7,  
 2,4-Pyrimidinediamine, 6-chloro-N4-(3-methylphenyl)- 6633-66-5,  
 2,4,6-Pyrimidinetriamine, N4-(4-bromophenyl)- 6807-82-5, L-Glutamic

[1,2,4]Triazolo[1,5-a]pyrimidine, 5,7-dimethyl-2-[(phenylmethyl)thio]-  
51893-98-2, Benzoic acid, 2-hydroxy-, [2-[(5-ethyl-1,4-dihydro-6-methyl-4-  
oxo-2-pyrimidinyl)thio]-1-phenylethylidene]hydrazide 51934-26-0,  
L-Glutamic acid, N-[4-[(7-amino-1,5-dihydro-5-thioxopyrimido[5,4-e]-1,2,4-  
triazin-3-yl)methyl]amino]benzoyl]-, diethyl ester, monohydrochloride  
51934-28-2, L-Glutamic acid, N-[4-[(5,7-diaminopyrimido[5,4-e]-1,2,4-  
triazin-3-yl)methyl]amino]benzoyl]-, diethyl ester 54299-50-2,  
2-Propen-1-one, 1-(2,4-dihydroxy-3,6-dimethoxyphenyl)-3-phenyl-  
54395-52-7, 1H-Isoindole-1,3(2H)-dione, 5,5'-[(1-methylethylidene)bis(4,1-  
phenyleneoxy)]bis[2-methyl- 56025-86-6, 1H-Purine-2,6-dione,  
3,7-dihydro-3-methyl-7-(phenylmethyl)- 56307-99-4, Ethanone,  
1-(2,4-dihydroxyphenyl)-2-(phenylthio)- 57710-80-2, 1H-Benzotriazole-1-  
carboxylic acid, phenylmethyl ester 57808-66-9, 2H-Benzimidazol-2-one,  
5-chloro-1-[1-[3-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)propyl]-4-  
piperidinyl]-1,3-dihydro- 57966-42-4, L-Threonine, L-arginyl-L-tyrosyl-L-  
leucyl-L-prolyl- 58677-09-1, L-Glutamic acid, N-[4-[(2-amino-1,4-  
dihydro-4-oxo-6-quinazolinyl)methyl]methylamino]benzoyl]-, diethyl ester  
60045-61-6, 4,6(1H,5H)-Pyrimidin-2-one, dihydro-5-[(4-  
methoxyphenyl)methylene]-2-thio- 60407-48-9, L-Isoleucine,  
L-arginylglycyl-L-prolyl-L-phenylalanyl-L-prolyl- 60482-96-4, L-Leucine,  
L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- 61043-53-6,  
L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-alanyl-N-(4-  
nitrophenyl)- 64792-21-8, 2-Propenal, 3-phenyl-, (1,4-dihydro-6-methyl-4-  
oxo-2-pyrimidinyl)hydrazone 64801-58-7, L-Aspartic acid,  
N-[4-[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]-L-γ-  
glutamyl- 65147-09-3, L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L-  
leucylglycyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)- 65757-04-2,  
L-Glutamic acid, N-[4-[(1,2,3,4-tetrahydro-2-imino-1,3-dimethyl-4-oxo-6-  
pteridinyl)methyl]amino]benzoyl]-, dimethyl ester 65757-05-3, L-Glutamic  
acid, N-[4-[(2-amino-3,4-dihydro-3-methyl-4-oxo-6-  
pteridinyl)methyl]amino]benzoyl]-, dimethyl ester 65877-43-2D,  
1,3-Benzenediol, 5-[2-(3-hydroxy-4-methoxyphenyl)ethenyl]-, glycoside  
derivative 66048-53-1, Guanosine, 2',3',5'-tribenzoate 66147-31-7,  
L-Glutamic acid, N-[4-[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzo-  
yl]-, 5-butyl ester 67368-29-0, L-Alanine, L-methionyl-L-arginyl-L-  
phenylalanyl- 67655-19-0, Phenol, 2,2'-[(2-hydroxy-1,3-  
propanediyl)bis(oxy)]bis- 67836-16-2, Acetamide, 2-(2,4-dichlorophenoxy)-  
N-1H-1,2,4-triazol-3-yl- 68047-41-6, 1,3,4-Oxadiazole,  
2-(3-bromophenyl)-5-(2-naphthalenyl)- 68215-68-9, Phenol,  
2-[4-amino-6-[(4-chlorophenyl)amino]-1,3,5-triazin-2-yl]-4-chloro-  
68682-02-0, 4H-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-(4-  
hydroxyphenyl)-8-(3-methyl-2-butenyl)- 68838-40-4, 1H-1,2,4-Triazole,  
3-methyl-5-[(phenylmethyl)thio]- 69097-98-9, 4H-1-Benzopyran-4-one,  
2,3-dihydro-5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)- 69193-20-0,  
4-Pyrimidinamine, 5-bromo-N-phenyl- 69480-15-5, 3H-1,2,4-Triazole-3-  
thione, 5-[4-(1,1-dimethylethyl)phenyl]-1,2-dihydro- 70280-72-7,  
L-Glutamic acid, N-[4-[(2,4-diamino-6-pteridinyl)methyl](phenylmethyl)ami-  
no]benzoyl]-, diethyl ester 70280-75-0, L-Glutamic acid,  
N-[4-[(2,4-diamino-6-pteridinyl)methyl]ethylamino]benzoyl]-, diethyl  
ester 70539-54-7, L-Glutamic acid, N-[3,5-dichloro-4-[(2,4-diamino-6-  
pteridinyl)methyl]ethylamino]benzoyl]-, diethyl ester 70968-04-6,  
L-Leucinamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-alanyl-L-prolyl-N-(4-  
nitrophenyl)- 71047-38-6, 1H-Imidazole, 1-(3,7-dimethyl-2,6-octadienyl)-  
71074-46-9, Glycine, N-[N-[4-[(2,4-diamino-6-  
pteridinyl)methyl]methylamino]benzoyl]-L-γ-glutamyl]- 71074-48-1,  
L-Aspartic acid, N-[4-[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzo-  
yl]-L-α-glutamyl- 71074-49-2, L-Glutamic acid,  
N-[4-[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]-L-α-  
glutamyl- 71707-02-3, L-Glutamic acid, N-[N-[4-[(2,4-diamino-6-

prolyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)-, phenylmethyl ester  
 113866-16-3, L-Argininamide, N-[(1,1-dimethylethoxy)carbonyl]-L- $\alpha$ -  
 glutamyl-L-alanyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)-, phenylmethyl  
 ester 117889-48-2, 1H-Tetrazole, 5-[(2,4-dichlorophenoxy)methyl]-  
 118034-92-7, L-Threonine, L-histidyl-L-phenylalanyl-L-methionyl-L-prolyl-  
 120225-54-9, Benzenepropanoic acid, 4-[2-[[6-amino-9-(N-ethyl- $\beta$ -D-  
 ribofuranuronamidosyl)-9H-purin-2-yl]amino]ethyl]- 121036-80-4,  
 1,2,4-Triazin-5(2H)-one, 6-[2-(4-methylphenyl)ethenyl]-3-phenyl-  
 121036-81-5, 1,2,4-Triazin-5(2H)-one, 6-[2-(4-methoxyphenyl)ethenyl]-3-  
 phenyl- 124485-41-2, L-Argininamide, N-[(phenylmethoxy)carbonyl]-L-valyl-  
 L-valyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)- 126235-09-4,  
 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(2-phenylethyl)-  
 128802-79-9, L-Phenylalaninamide, N-(3-carboxy-1-oxopropyl)-L-alanyl-L-  
 isoleucyl-L-prolyl-N-(4-nitrophenyl)- 131061-65-9, 7H-Purine-7-butanoic  
 acid, 1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-8-[(phenylmethyl)amino]-,  
 ethyl ester 132467-01-7, 2(1H)-Quinoxalinone, 3-[2-(2-  
 chlorophenyl)ethenyl]- 133061-57-1, 2,4-Pyrimidinediamine,  
 N4-(3,5-dichlorophenyl)-6-methyl- 134759-22-1, 1H-Thieno[3,4-d]imidazole-  
 4-pentanamide, N-[6-[[5-[[[3',6'-dihydroxy-3-oxospiro[isobenzofuran-  
 1(3H),9']-[9H]xanthen]-5-yl]amino]thioxomethyl]amino]pentyl]amino]-6-  
 oxohexyl]hexahydro-2-oxo-, (3aS,4S,6aR)- 134796-34-2, 1H-1,2,4-Triazole,  
 3-[[[(4-chlorophenyl)methyl]thio]- 137484-84-5, 1,3,5-Triazin-2-amine,  
 4-chloro-6-[3-(2-furanyl)propoxy]-N,N-dimethyl- 137833-31-9,  
 Myelo peptide 2 138194-56-6, 1H-Pyrrole-2,5-dione, 1-[3-[[[(4-oxo-1,2,3-  
 benzotriazin-3(4H)-yl)oxy]carbonyl]phenyl]- 138915-75-0, L-Leucine,  
 N-acetyl-L-histidyl-L-tryptophyl-L-alanyl-L-valylglycyl-L-histidyl-  
 142206-40-4, 1H-Benzimidazole, 2,2'-(1,3-propanediyl)bis[1-methyl-  
 143113-41-1, L-Valine, L-Histidyl-L-Alanyl 146871-70-7,  
 4-Quinazolinamine, N-(3-chlorophenyl)-, monohydrochloride 148337-06-8,  
 Glycine, L-prolylglycyl-L-alanyl-L-isoleucyl-L-prolyl- 151358-70-2,  
 2-Propen-1-one, 1,1'-(2,6-pyridinediyl)bis[3-(4-hydroxyphenyl)-  
 152028-96-1, 1H-Imidazole, 4-[3-[(4-iodophenyl)methoxy]propyl]-  
 154719-25-2, L-Lysinamide, N-acetyl-L-tyrosyl-L-valyl-N-[(1S)-1-  
 (carboxymethyl)-3-[(2,6-dimethylbenzoyl)oxy]-2-oxopropyl]-N6-[5-  
 [(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]-  
 155373-59-4, 4H-1-Benzopyran-4-one, 3-[[4-(1H-tetrazol-5-yl)phenyl]methyl]-  
 155373-72-1, 4H-1-Benzopyran-4-one, 2-phenyl-7-[4-(1H-tetrazol-5-  
 yl)butoxy]- 160347-57-9D, 2(1H)-Pyrimidinone, 5-(4-pentylphenyl)-,  
 derivs. 185503-97-3, L-Lysine, N6-[[4-[[4-(dimethylamino)phenyl]azo]phen  
 yl]sulfonyl]-N2-[(9H-fluoren-9-ylmethoxy)carbonyl]- 188966-22-5D,  
 Phenol, 2-(2H-benzotriazol-2-yl)-4-(1,1-dimethylhexyl)-, derivs.  
 191411-47-9, 1H-Imidazole-5-methanol, 1-methyl-2-[(phenylmethyl)thio]-  
 194424-08-3, Glutamic acid, N-[4-[[3-(2-thienyl)-2-  
 quinoxaliny]amino]benzoyl]-, dipropyl ester 195140-70-6, 1H-Imidazole,  
 1-[2-(phenylmethoxy)ethyl]- 196600-87-0, Tyrosine, N-  
 [(phenylmethoxy)carbonyl]norvalylglycyl-, methyl ester 197456-56-7,  
 1,4-Naphthalenedione, 2-[4-(decahydro-2-naphthalenyl)butyl]-3-hydroxy-  
 198488-04-9, Urea, N,N'-(3,3'-dimethyl[1,1'-biphenyl]-4,4'-diyl)bis[N'-(2-  
 methylphenyl)- 198632-08-5, L-Proline, glycyl-L-arginylglycyl-L- $\alpha$ -  
 glutamyl-L-threonyl- 199929-21-0, 1,4-Naphthalenedione,  
 2-hydroxy-3-[8-(4-methylphenoxy)octyl]- 200058-34-0,  
 1,4-Naphthalenedione, 2-(3-[1,1'-bicyclohexyl]-4-ylpropyl)-3-hydroxy-  
 200061-22-9, Phenol, 4,4'-(1-methylethylidene)bis-, bis(3,5-  
 dinitrobenzoate) 200431-98-7, 3-Pyridinemethanamine,  
 N-1H-1,2,4-triazol-3-yl- 200505-51-7, Decanedioic acid,  
 bis[[4-(ethoxy-3-methoxyphenyl)methylene]hydrazide] 200706-30-5,  
 4H-1,2,4-Triazol-4-amine, N-[(2,3-dihydro-1H-inden-5-yl)methylene]-  
 200706-45-2, 4-Imidazolidinone, 5-[(2,3-dihydro-1H-inden-5-yl)methylene]-2-  
 thioxo- 201997-13-9, 1,3-Benzenediol, 4-[[[2-hydroxy-2-(4-

HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,  
 LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,  
 SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,  
 YU, ZA, ZW  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
 BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2000-491078 A 20000124 <--

OTHER SOURCE(S): MARPAT 135:147398

AB Peptidomimetics of cyclic peptides, and compns. comprising such  
 peptidomimetics are provided. The peptidomimetics have a three-dimensional  
 structure that is substantially similar to a three-dimensional structure of a  
 cyclic peptide that comprises a cadherin cell adhesion recognition sequence  
 HAV. Methods for using such peptidomimetics for modulating cadherin-mediated  
 cell adhesion in a variety of contexts are also provided.

IC ICM C07K007-00

CC 1-3 (Pharmacology)

Section cross-reference(s): 34, 63

IT Antitumor agents

Bioreactors

Bond angle

Cell migration

Combinatorial library

Drug delivery systems

Drug screening

Drug targeting

Electrostatic charge

Epithelium

Hydrophobicity

Melanoma

Membrane, biological

Microparticles

Molecular modeling

Multiple sclerosis

Oligodendrocyte

Ovary, neoplasm

Peptidomimetics

Protein sequences

QSAR (structure-activity relationship)

Schwann cell

Steric effects

Transplant and Transplantation

Transplant and Transplantation

Ultrathin films

Wound healing

Wound healing promoters

(peptidomimetic modulators of cell adhesion)

IT 57-88-5D, Cholest-5-en-3-ol (3 $\beta$ )-, glycoside derivs. 135-16-0

487-49-0 548-73-2 570-88-7 1210-66-8 1482-74-2 1699-40-7

1776-30-3 2486-02-4 2810-37-9 2979-51-3 3242-68-0 3257-73-6

3561-56-6 3566-25-4 3575-07-3 3922-47-2 4672-96-2 5226-71-1

5341-00-4 5415-88-3 5421-95-4 5426-87-9 5429-46-9 5446-36-6

5454-50-2 5454-52-4 5508-58-7 5534-95-2 5786-82-3 5800-34-0

6286-57-3 6295-27-8 6300-80-7 6320-71-4 6322-09-4 6323-88-2

6323-89-3 6331-03-9 6338-84-7 6340-76-7 6633-66-5 6807-82-5

6962-62-5 6975-34-4 7781-29-5 10320-97-5 13184-14-0 13351-10-5

13745-20-5 15013-60-2 15970-42-0 16856-21-6 16879-84-8

17357-75-4 17430-65-8 17496-31-0 18100-11-3 18100-12-4

18211-37-5 19312-13-1 19484-75-4D, furanoside derivative 19889-31-7

20621-49-2 21108-76-9 21658-45-7 23567-67-1 23815-88-5,

## STRUCTURE + ASSAY

=&gt; d que nos 1141; d que nos 1146; d que nos 1148

L42 SCR 1839 AND 1993  
 L50 STR  
 L52 SCR 392 OR 391  
 L73 SCR 1952  
 L81 57965 SEA FILE=REGISTRY SSS FUL (L50) AND L42 AND L52 AND L73  
 L84 53736 SEA FILE=REGISTRY SSS FUL (L50) AND L42 AND L52 NOT L73  
 L85 111701 SEA FILE=REGISTRY ABB=ON (L81 OR L84)  
 L87 STR  
 L88 STR  
 L89 STR  
 L90 STR  
 L93 8317 SEA FILE=REGISTRY SUB=L85 SSS FUL (L50 NOT (L87 OR L88 OR L89  
 OR L90))  
 L94 1407 SEA FILE=HCAPLUS ABB=ON L93  
 L130 912 SEA FILE=HCAPLUS ABB=ON L94 AND (PY<2001 OR AY<2001 OR  
 PRY<2001)  
 L140 131348 SEA FILE=HCAPLUS ABB=ON ASSAY?/OBI  
 L141 2 SEA FILE=HCAPLUS ABB=ON L130 AND L140

L42 SCR 1839 AND 1993  
 L50 STR  
 L52 SCR 392 OR 391  
 L73 SCR 1952  
 L81 57965 SEA FILE=REGISTRY SSS FUL (L50) AND L42 AND L52 AND L73  
 L84 53736 SEA FILE=REGISTRY SSS FUL (L50) AND L42 AND L52 NOT L73  
 L85 111701 SEA FILE=REGISTRY ABB=ON (L81 OR L84)  
 L87 STR  
 L88 STR  
 L89 STR  
 L90 STR  
 L93 8317 SEA FILE=REGISTRY SUB=L85 SSS FUL (L50 NOT (L87 OR L88 OR L89  
 OR L90))  
 L94 1407 SEA FILE=HCAPLUS ABB=ON L93  
 L130 912 SEA FILE=HCAPLUS ABB=ON L94 AND (PY<2001 OR AY<2001 OR  
 PRY<2001)  
 L142 269019 SEA FILE=HCAPLUS ABB=ON FLUORESCEN?/OBI  
 L144 687360 SEA FILE=HCAPLUS ABB=ON ?ASSAY?/BI  
 L146 9 SEA FILE=HCAPLUS ABB=ON L130 AND L142 AND L144

L42 SCR 1839 AND 1993  
 L50 STR  
 L52 SCR 392 OR 391  
 L73 SCR 1952  
 L81 57965 SEA FILE=REGISTRY SSS FUL (L50) AND L42 AND L52 AND L73  
 L84 53736 SEA FILE=REGISTRY SSS FUL (L50) AND L42 AND L52 NOT L73  
 L85 111701 SEA FILE=REGISTRY ABB=ON (L81 OR L84)  
 L87 STR  
 L88 STR  
 L89 STR  
 L90 STR  
 L93 8317 SEA FILE=REGISTRY SUB=L85 SSS FUL (L50 NOT (L87 OR L88 OR L89  
 OR L90))  
 L94 1407 SEA FILE=HCAPLUS ABB=ON L93

(Photosensitizer and sensitizers; amplified luminescent homogeneous immunoassay)

IT Ethers, uses  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (Seleno; amplified luminescent homogeneous immunoassay)

IT Ethers, uses  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (Telluro; amplified luminescent homogeneous immunoassay)

IT Alcohols, uses  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (alkoxy, p-; amplified luminescent homogeneous immunoassay)

IT Reaction  
 (amplification; amplified luminescent homogeneous immunoassay  
 )

IT Binders  
 Chemical formula  
 Composition  
 Electron transfer catalysts  
 Fluorescence  
 Fluorescence quenching  
 Fluorescent indicators  
 Light  
 Mixtures  
 Molecular association  
 Molecules  
 Oxidizing agents  
 Radiation  
 Radioimmunoassay  
 Reaction  
 Test kits  
 Wavelength  
 (amplified luminescent homogeneous immunoassay)

IT Nucleic acids  
 RL: ANT (Analyte); ANST (Analytical study)  
 (amplified luminescent homogeneous immunoassay)

IT Polynucleotides  
 RL: ANT (Analyte); ARG (Analytical reagent use); ANST (Analytical study);  
 USES (Uses)  
 (amplified luminescent homogeneous immunoassay)

IT Alkenes, uses  
 Antibodies and Immunoglobulins  
 Aromatic compounds  
 Avidins  
 Disulfides  
 Enamines  
 Enzymes, uses  
 Ligands  
 Thioethers  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (amplified luminescent homogeneous immunoassay)

IT Reactive oxygen species  
 RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)  
 (amplified luminescent homogeneous immunoassay)

IT Oligonucleotides  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (amplified luminescent homogeneous immunoassay)

IT Polymerization  
 (co-; amplified luminescent homogeneous immunoassay)

IT Ethers, uses  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)

Bis-Phenyl)Ethynyl Anthracene 601480-97-1 753000-95-2 753001-01-3  
753038-52-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
(amplified luminescent homogeneous immunoassay)

IT 5455-98-1DP, reaction products with dextran, beads coated with  
90360-25-1P 146425-95-8P 185017-15-6P 185017-16-7P 753000-91-8P  
753000-92-9P 753000-96-3P 753000-99-6P 753001-00-2P 753001-05-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(amplified luminescent homogeneous immunoassay)

IT 58-85-5DP, Biotin, O-acyl derivs. 4442-17-5P, 3-Ketodigoxigenin  
9004-54-0DP, Dextran, hydroxypropylamino derivs. coated beads  
151802-91-4P 193027-49-5DP, beads coated with, reaction products with  
hydrazine 193027-49-5P 753000-93-0P 753000-94-1P 753000-97-4P  
753000-98-5P 753001-02-4P 753001-03-5P 753001-06-8P 753001-13-7P  
RL: SPN (Synthetic preparation); PREP (Preparation)

(amplified luminescent homogeneous immunoassay)

IT 20830-75-5, Digoxin

RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(monoclonal antibody to; amplified luminescent homogeneous  
immunoassay)

IT 7782-44-7, Oxygen, reactions

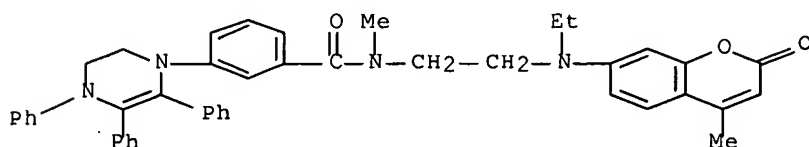
RL: FMU (Formation, unclassified); RCT (Reactant); FORM (Formation,  
nonpreparative); RACT (Reactant or reagent)  
(singlet; amplified luminescent homogeneous immunoassay)

IT 753001-07-9

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
(amplified luminescent homogeneous immunoassay)

RN 753001-07-9 HCAPLUS

CN Benzamide, 3-(3,4-dihydro-4,5,6-triphenyl-1(2H)-pyrazinyl)-N-[2-[ethyl(4-  
methyl-2-oxo-2H-1-benzopyran-7-yl)amino]ethyl]-N-methyl- (9CI) (CA INDEX  
NAME)



L165 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:643488 HCAPLUS Full-text

DOCUMENT NUMBER: 133:360325

TITLE: A fluorescence-quenched chitopentaose for  
the study of endo-chitinases and chitobiosidases

AUTHOR(S): Cottaz, Sylvain; Brasme, Bernard; Driguez, Hugues

CORPORATE SOURCE: Centre de Recherches sur les Macromolécules Végétales,  
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DOCUMENT TYPE: Journal

LANGUAGE: English

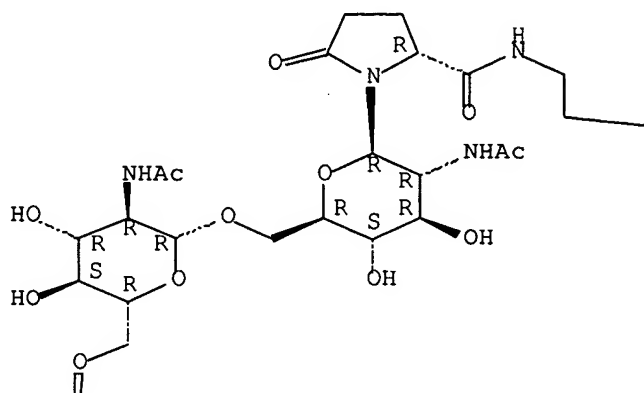
AB A new fluorogenic substrate displaying intramol. fluorescence energy transfer  
(FRET) has been synthesized from NI,NII,NIII,NIV-tetra-acetyl- chitopentaose.



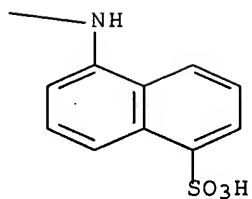
glucopyranosyl-(1→6)-O-2-(acetyl amino)-2-deoxy-β-D-  
 glucopyranosyl-(1→6)-O-2-(acetyl amino)-2-deoxy-β-D-  
 glucopyranosyl-(1→6)-2-(acetyl amino)-2-deoxy-β-D-  
 glucopyranosyl]-5-oxo-2-pyrrolidinyl]carbonyl]amino]ethyl]amino]- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry unknown.

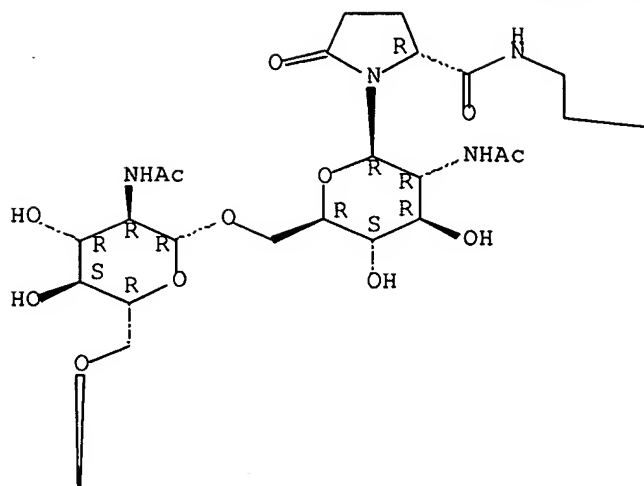
PAGE 1-A



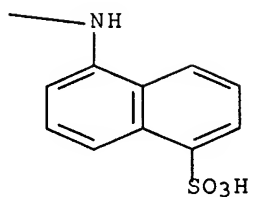
PAGE 1-B



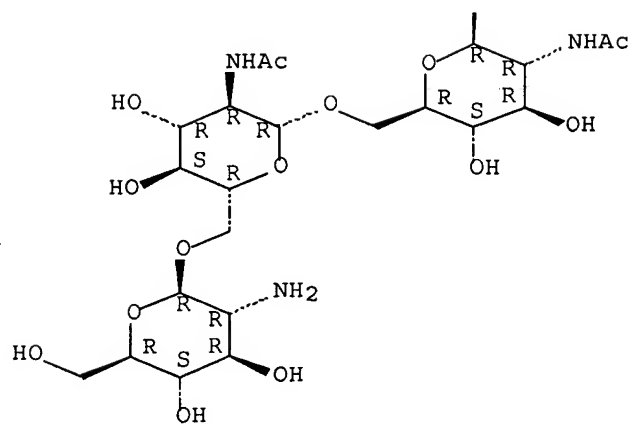
PAGE 1-A



PAGE 1-B



PAGE 2-A



REFERENCE COUNT:

35

THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS

unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process)

(quenching fluoroimmunoassay for anal. of the pesticide propazine in an apolar organic solvent, reverse micelles of AOT in n-octane)

IT 163405-32-1 163405-33-2 163405-34-3 203194-80-3  
203194-81-4 203194-82-5 203194-83-6

RL: ARU (Analytical role, unclassified); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); PROC (Process)

(quenching fluoroimmunoassay for anal. of the pesticide propazine in an apolar organic solvent, reverse micelles of AOT in n-octane)

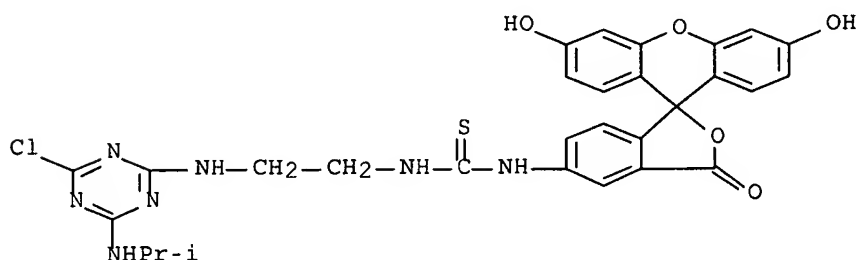
IT 163405-32-1 203194-82-5

RL: ARU (Analytical role, unclassified); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); PROC (Process)

(quenching fluoroimmunoassay for anal. of the pesticide propazine in an apolar organic solvent, reverse micelles of AOT in n-octane)

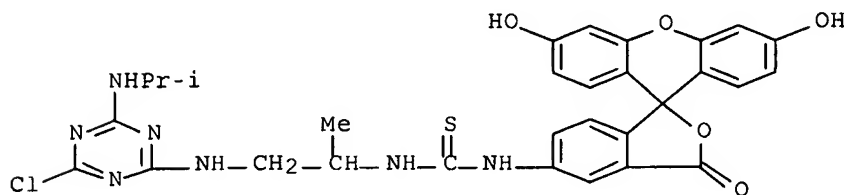
RN 163405-32-1 HCAPLUS

CN Thiourea, N-[2-[[4-chloro-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]amino]ethyl]-N'-(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)- (CA INDEX NAME)



RN 203194-82-5 HCAPLUS

CN Thiourea, N-[2-[[4-chloro-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]amino]-1-methylethyl]-N'-(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)- (CA INDEX NAME)



REFERENCE COUNT:

19

THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L165 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:401614 HCAPLUS Full-text

DOCUMENT NUMBER: 125:53030

IT Antibodies  
 Avidins  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (double-stranded nucleic acids as universal link system in  
 immunoassays)

IT Immunoassay  
 (chemiluminescence, double-stranded nucleic acids as universal link  
 system in immunoassays)

IT 50-06-6, Phenobarbital, analysis 58-55-9, Theophylline, analysis  
 9002-71-5, TSH  
 RL: ANT (Analyte); ANST (Analytical study)  
 (double-stranded nucleic acids as universal link system in  
 immunoassays)

IT 58-85-5, Biotin 178255-26-0 178255-29-3 178255-32-8  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (double-stranded nucleic acids as universal link system in  
 immunoassays)

IT 178255-24-8DP, conjugates 178255-25-9DP, conjugates 178255-27-1DP,  
 conjugates 178255-28-2DP, conjugates 178255-30-6DP, conjugates  
 178255-31-7DP, conjugates 178318-53-1P 178318-54-2P  
 178359-42-7DP, Fractogel OH, oligonucleotide conjugates  
 RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST  
 (Analytical study); PREP (Preparation); USES (Uses)  
 (double-stranded nucleic acids as universal link system in  
 immunoassays)

IT 57-13-6, Urea, analysis 75-12-7, Formamide, analysis 9004-34-6D,  
 Cellulose, poly dA conjugates  
 RL: ARU (Analytical role, unclassified); ANST (Analytical study)  
 (double-stranded nucleic acids as universal link system in  
 immunoassays)

IT 14808-60-7, Quartz, analysis  
 RL: ARU (Analytical role, unclassified); DEV (Device component use); ANST  
 (Analytical study); USES (Uses)  
 (double-stranded nucleic acids as universal link system in  
 immunoassays)

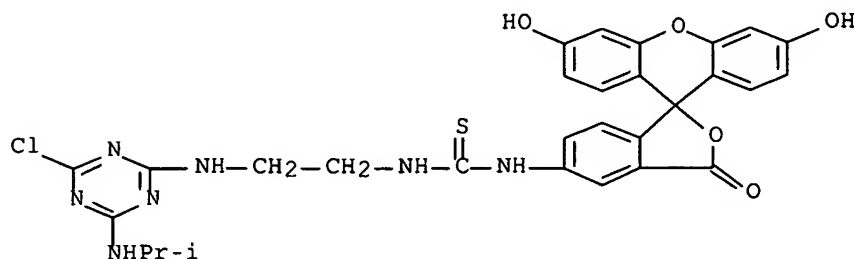
IT 4044-65-9, 1,4-Phenylene diisothiocyanate 27072-45-3, FITC 103708-09-4  
 178318-55-3 178318-56-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (double-stranded nucleic acids as universal link system in  
 immunoassays)

IT 178318-54-2P  
 RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST  
 (Analytical study); PREP (Preparation); USES (Uses)  
 (double-stranded nucleic acids as universal link system in  
 immunoassays)

RN 178318-54-2 HCAPLUS

CN Thiourea, N-(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-  
 [9H]xanthen]-5-yl)-N'-[2-[(2,3,6,7-tetrahydro-1,3-dimethyl-2,6-dioxo-1H-  
 purin-8-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

CN Thiourea, N-[2-[[4-chloro-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]amino]ethyl]-N'-(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-(9H)xanthen]-5-yl)- (CA INDEX NAME)



L165 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1991:82496 HCAPLUS Full-text  
 DOCUMENT NUMBER: 114:82496  
 TITLE: Design and synthesis of new fluorogenic HIV protease substrates based on resonance energy transfer  
 AUTHOR(S): Wang, Gary T.; Matayoshi, Edmund; Huffaker, H. Jan; Krafft, Grant A.  
 CORPORATE SOURCE: Abbott Lab., Abbott Park, IL, 60064-3500, USA  
 SOURCE: Tetrahedron Letters (1990), 31(45), 6493-6  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 114:82496  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The design and synthesis of new fluorogenic substrate probes for HIV protease based on resonance energy transfer are described. These substrates permit sensitive, continuous measurement of HIV protease activity. Thus, Gaba derivative I was coupled with H-Ser-Gln-Asn-Tyr-Pro-Ile-Val-Gln-OH to give the acyl peptide, which was coupled with naphthalenesulfonic acid derivative II by EDC/N-hydroxysuccinimide to give title fluorogenic peptide derivative III. I is cleaved specifically at the Tyr-Pro amide bond by HIV protease. Addition of purified recombinant HIV-1 protease to the substrate results in a steady increase in fluorescence intensity, permitting continuous monitoring of the enzyme activity. Exhaustive proteolysis of I produces a 40-fold fluorescence enhancement above the background fluorescence level, imparting to this assay the highest sensitivity of any method used to measure HIV protease activity.

CC 34-3 (Amino Acids, Peptides, and Proteins)  
 Section cross-reference(s): 9, 10

IT Fluorescence  
 (of human immunodeficiency virus protease substrate)

IT 131941-76-9 131941-77-0 131941-78-1  
 RL: PRP (Properties)  
 (fluorescence of)

IT 131941-78-1  
 RL: PRP (Properties)

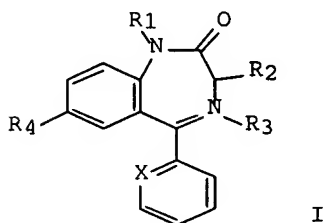
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EP 264797	A3	19900207		
EP 264797	B1	19960110		
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ES 2084577	T3	19960516	ES 1987-114982	19871014 <--
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AU 643490	B2	19931118		

PRIORITY APPLN. INFO.:

US 1986-922595	A	19861024 <--
AU 1987-79975	A	19871021 <--

OTHER SOURCE(S): MARPAT 110:91693

GI



AB Benzodiazepine derivs. I [X = CH, N, C-halogen; R1 = H, Me, RZQ; R2 = H, OH; R3 = O or nonbonding electron pair; R4 = RZQ when R1 = H, Me or R4 = halogen, NO2, NH2, NHCOMe when R1 = RZQ; R = linking group containing 0-20 C and heteroatoms ( $\leq 12$ ), arranged in a straight or branched chain and containing  $\leq 2$  rings and  $\leq 4$  heteroatoms and  $\leq 2$  S or N or 1 O may be linked in sequence; Z = CO, CNH, NH, NMe, N2, SO2, CH2; Q = H, OH, halogen, acyloxy, N-succinimidyloxy, N-phthalimidyloxy, alkoxy, (substituted) phenoxy, N-imidazolyl, 1-benzotriazolyl, poly(amino acid) (derivative), immunogenic carrier, or amino, amido, anidino, (thio) urea, (thio) carbamate, triazinylamino, or (carboxyamino)-sulfonamido derivative of fluorescein] are prepared as precursors, immunogens, or tracers for a fluorescence-polarization immunoassay for determining the presence or amount of benzodiazepines and their metabolites in a sample. An immunogen was prepared by coupling 1-carboxymethyl-7-chloro-1,3-dihydro-5-phenyl-2H-1,4-benzodiazepin-2-one with bovine serum albumin via dicyclohexylcarbodiimide and N-hydroxysuccinimide.

IC ICM G01N033-531

ICS G01N033-533; G01N033-542

CC 9-14 (Biochemical Methods)

Section cross-reference(s): 1

ST benzodiazepine fluorescence polarization immunoassay;  
 fluorescein benzodiazepine deriv conjugate immunoassay; albumin  
 benzodiazepine deriv conjugate immunogen

IT Antigens

RL: ANST (Analytical study)  
 (benzodiazepine derivs.-albumin conjugates as, for fluorescence  
 -polarization immunoassay)

IT Antiserums

Antibodies

RL: ANST (Analytical study)

conjugates 119194-55-7DP, benzodiazepine derivative conjugates

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, for fluorescence-polarization immunoassay for benzodiazepines and metabolites)

IT 1088-11-5 4959-16-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in synthesis of immunogen for fluorescence-polarization immunoassay for benzodiazepines)

IT 107-15-3, 1,2-Ethanediamine, reactions 75178-70-0 105064-28-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in synthesis of precursor for immunogen or tracer for fluorescence-polarization immunoassay for benzodiazepines)

IT 4959-16-4 119215-05-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in synthesis of tracer for fluorescence-polarization immunoassay for benzodiazepines)

IT 2916-68-9, 2-(Trimethylsilyl)ethanol 27072-45-3, Fluoresceinisothiocyanate 27599-63-9, Amino fluorescein 51306-35-5

82169-58-2 92557-81-8 106754-95-4 119181-21-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with benzodiazepine derivative in preparation of tracer for fluorescence-polarization immunoassay)

IT 119194-43-3 119194-44-4

RL: ANST (Analytical study)

(tracer for fluorescence-polarization immunoassay for benzodiazepines)

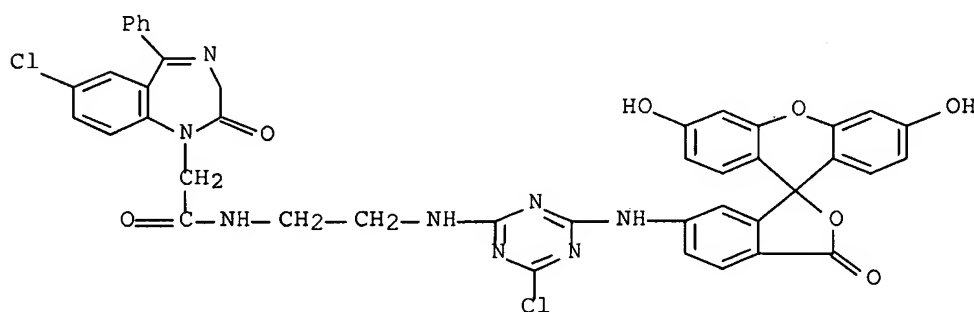
IT 119194-43-3

RL: ANST (Analytical study)

(tracer for fluorescence-polarization immunoassay for benzodiazepines)

RN 119194-43-3 HCAPLUS

CN 1H-1,4-Benzodiazepine-1-acetamide, 7-chloro-N-[2-[[4-chloro-6-[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl)amino]-1,3,5-triazin-2-yl]amino]ethyl]-2,3-dihydro-2-oxo-5-phenyl- (CA INDEX NAME)



L165 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1988:180109 HCAPLUS Full-text

DOCUMENT NUMBER: 108:180109

TITLE: Preparation of tracers for use in flecainide fluorescence polarization immunoassay

INVENTOR(S): Heiman, Daniel Feulner

PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: Eur. Pat. Appl., 36 pp.

tracer; fluoresceinylaminotriazine deriv immunoassay flecainide;  
aminotriazine fluoresceinyl deriv immunoassay flecainide

IT 54143-55-4, Flecainide

RL: ANT (Analyte); ANST (Analytical study)

(determination of, by fluorescence-polarization immunoassay  
, tracers for)

IT 114258-03-6P 114258-04-7P 114258-05-8P 114258-06-9P 114258-07-0P  
114258-08-1P 114258-09-2P 114258-10-5P 114258-11-6P  
114258-12-7P 114258-13-8P 114258-14-9P 114258-15-0P  
114258-16-1P 114258-17-2P 114258-18-3P 114258-19-4P 114258-20-7P  
114282-72-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as tracer for flecainide fluorescence  
-polarization immunoassay)

IT 2321-07-5, Fluorescein 2321-07-5D, Fluorescein, derivs. 3326-34-9,  
5-Aminofluorescein 51306-35-5 51649-83-3, 6-Aminofluorescein  
82169-58-2 92557-81-8 114258-21-8 114258-23-0 114258-24-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with flecainide derivs. in preparation of tracers for  
fluorescence-polarization immunoassays)

IT 54143-55-4D, Flecainide, derivs. 54143-56-5, Flecainide acetate  
114258-22-9 114258-25-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with fluorescein derivs. in preparation of tracers for  
fluorescence-polarization immunoassays)

IT 114258-12-7P

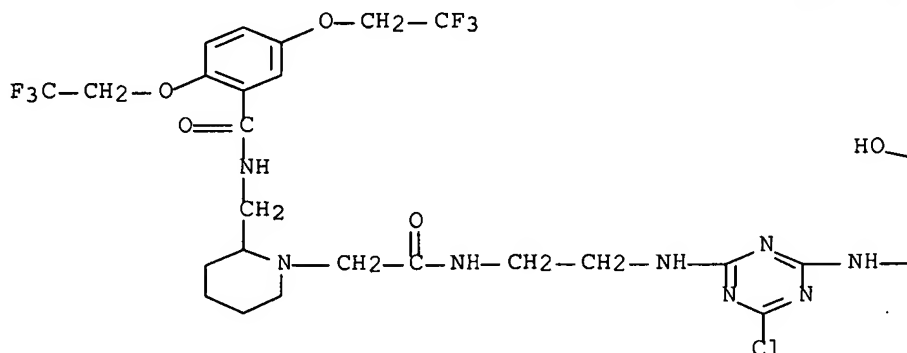
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as tracer for flecainide fluorescence  
-polarization immunoassay)

RN 114258-12-7 HCAPLUS

CN 1-Piperidineacetamide, 2-[[[2,5-bis(2,2,2-trifluoroethoxy)benzoyl]amino]me  
thyl]-N-[2-[[[4-chloro-6-[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-  
1(3H),9']-[9H]xanthen)-6-yl)amino]-1,3,5-triazin-2-yl]amino]ethyl]- (CA  
INDEX NAME)

PAGE 1-A





US 1988-90001614 A 19881005 &lt;--

OTHER SOURCE(S): MARPAT 100:206160

- AB A fluorescent polarization immunoassay and reagents are described for the determination of ligands (e.g., steroids, hormones, anticonvulsants, antibiotics, etc.) in biol. fluids. The reagent consists of a biol. acceptable salt (e.g., Na salt) of a triazinylaminofluorescein derivative with an attached ligand analog and a halo or lower alkyl analog. Thus, a reagent was prepared by reacting gentamicin sulfate (in water, pH 9.0) with 5-[(4,6-dichlorotriazin-2-yl)-amino]fluorescein (in MeOH) and the product was purified by DEAE-cellulose chromatog. The reagent was used for the determination of gentamicin in human serum or other biol. fluids.
- IC G01N033-54; G01N033-58; G01N033-52; G01N033-74
- INCL 436536000
- CC 9-2 (Biochemical Methods)  
Section cross-reference(s): 1, 2
- ST body fluid ligand detn immunoassay; fluorescence  
polarization immunoassay hormone; drug fluorescence  
polarization immunoassay serum; triazinylaminofluorescein deriv  
fluorescence polarization immunoassay
- IT Blood analysis  
(acetylprocainamide and gentamicin determination in, by fluorescence  
polarization immunoassay, reagents for)
- IT Antibiotics  
Antidepressants  
Pharmaceutical analysis  
(determination of, in biol. fluids by fluorescence polarization  
immunoassay, reagents for)
- IT Hormones  
Steroids, analysis  
RL: ANT (Analyte); ANST (Analytical study)  
(determination of, in biol. fluids by fluorescence polarization  
immunoassay, reagents for)
- IT Body fluid  
(ligands determination in, by fluorescence polarization  
immunoassay, reagents for)
- IT Immunochemical analysis  
(fluorescence-polarization immunoassay, for  
ligands)
- IT 50-47-5 50-49-7 51-48-9, analysis 56-54-2 56-75-7 57-41-0  
58-55-9, analysis 125-33-7 298-46-4 525-66-6 1404-04-2 3737-09-5  
20830-75-5  
RL: ANT (Analyte); ANST (Analytical study)  
(determination of, by fluorescence polarization immunoassay  
, reagents for)
- IT 50-06-6, analysis 50-47-5 50-48-6 50-49-7 51-06-9 56-54-2  
57-92-1, analysis 58-55-9, analysis 69-72-7, analysis 72-69-5  
99-66-1 1403-66-3 1404-90-6 32795-44-1 32986-56-4 37517-28-5  
RL: ANT (Analyte); ANST (Analytical study)  
(determination of, in biol. fluids by fluorescence polarization  
immunoassay, reagents for)
- IT 51306-35-5  
RL: ANST (Analytical study)  
(in fluorescence-polarization immunoassay)
- IT 57-92-1DP, reaction products with DTAF 1403-66-3DP, reaction products  
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reaction products with DTAF 37517-28-5DP, reaction products with DTAF  
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90275-41-5P 90275-42-6P 90275-43-7P 90275-44-8P 90275-45-9P  
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STRUCTURE + MICROMOLAR, EC50, Ki

=&gt; d que nos 1160; d que nos 1157; d que nos 1158

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L50          STR
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L73          SCR 1952
L81          57965 SEA FILE=REGISTRY SSS FUL (L50) AND L42 AND L52 AND L73
L84          53736 SEA FILE=REGISTRY SSS FUL (L50) AND L42 AND L52 NOT L73
L85          111701 SEA FILE=REGISTRY ABB=ON (L81 OR L84)
L87          STR
L88          STR
L89          STR
L90          STR
L93          8317 SEA FILE=REGISTRY SUB=L85 SSS FUL (L50 NOT (L87 OR L88 OR L89
              OR L90))
L94          1407 SEA FILE=HCAPLUS ABB=ON L93
L122         573 SEA FILE=HCAPLUS ABB=ON L94 (L) (THU OR BAC OR PAC OR PKT OR
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L160         4 SEA FILE=HCAPLUS ABB=ON L159 AND L130 AND L122

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L90          STR
L93          8317 SEA FILE=REGISTRY SUB=L85 SSS FUL (L50 NOT (L87 OR L88 OR L89
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L130         912 SEA FILE=HCAPLUS ABB=ON L94 AND (PY<2001 OR AY<2001 OR
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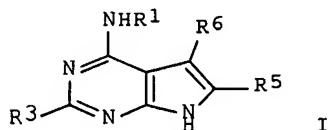
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 HK 1050319 A1 20070404 HK 2003-102257 20030328 <--  
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 US 1999-123216P P 19990308 <--  
 US 1999-126527P P 19990326 <--  
 WO 1999-US12135 A2 19990601 <--  
 US 1999-454074 A 19991202 <--  
 US 1999-454075 A 19991202 <--  
 US 1999-454254 A 19991202 <--  
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 OTHER SOURCE(S): MARPAT 142:392424  
 GI



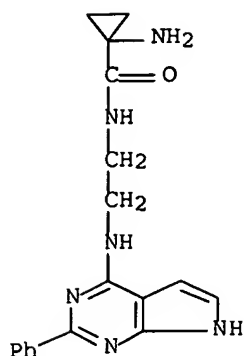
AB Title compds. [I; R1 = trans-4-hydroxycyclohexyl, 2-methylaminocarbonylaminoethyl, acetylaminoethyl, methylaminocarbonylaminoethyl; R3 = (substituted) Ph, pyrrolyl, thienyl, furyl, thiazolyl, imidazolyl, pyrazolyl, pyrazinyl, purinyl, quinazolinyl, etc.; R5 = H, (substituted) alkyl, amino, Ph, pyrrolyl, furyl, thienyl, imidazolyl, benzoxazolyl, benzothiazolyl, triazolyl, tetrazolyl, pyrazolyl, pyridinyl, pyrazinyl, pyridazinyl, pyrimidinyl, naphthyl, quinolyl, indolyl, etc.; R6 = H, (substituted) alkyl, cycloalkyl], were prepared Thus, 4-chloro-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine and trans-4-hydroxycyclohexylamine were heated in Me<sub>2</sub>SO at 130° for 5 h to give 75% 4-(4-trans-hydroxycyclohexyl)amino-6-methyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine. I showed A1 receptor binding with K<sub>i</sub> = 2.3-75000 nM..

IC ICM A61K031-517  
 ICS C07D239-94

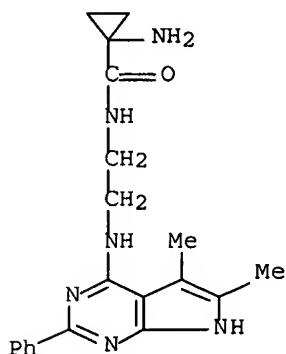
INCL 514264100; 544279000

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1, 63

IT 246855-41-4P 246855-42-5P 251945-90-1P 251945-91-2P 251945-93-4P  
 251945-94-5P 251945-95-6P 251945-96-7P 251945-97-8P 251945-98-9P  
 251945-99-0P 251946-01-7P 251946-02-8P 251946-06-2P 251946-07-3P  
 251946-08-4P 251946-10-8P 251946-11-9P 251946-12-0P 251946-13-1P  
 251946-14-2P 251946-15-3P 251946-16-4P 251946-17-5P 251946-18-6P  
 251946-19-7P 251946-20-0P 251946-21-1P 251946-22-2P 251946-23-3P  
 251946-24-4P 251946-25-5P 251946-26-6P 251946-27-7P  
 251946-28-8P 251946-29-9P 251946-30-2P 251946-31-3P 251946-32-4P  
 251946-33-5P 251946-34-6P 251946-35-7P 251946-36-8P 251946-37-9P  
 251946-38-0P 251946-39-1P 251946-40-4P 251946-41-5P 251946-42-6P  
 251946-43-7P 251946-44-8P 251946-45-9P 251946-46-0P 251946-47-1P  
 251946-48-2P 251946-49-3P 251946-50-6P 251946-52-8P 251946-53-9P



IT 343632-15-5  
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (preparation of aminopyrrolopyrimidines as adenosine A1 receptor antagonists)  
 RN 343632-15-5 HCAPLUS  
 CN Cyclopropanecarboxamide, 1-amino-N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl] - (9CI) (CA INDEX NAME)



REFERENCE COUNT: 120 THERE ARE 120 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L167 ANSWER 2 OF 21 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:88297 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 140:146159

TITLE: Preparation and use of substituted pyrrolo[2,3-d]pyrimidines as selective adenosine A3 receptor antagonists

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan; Witter, David J.

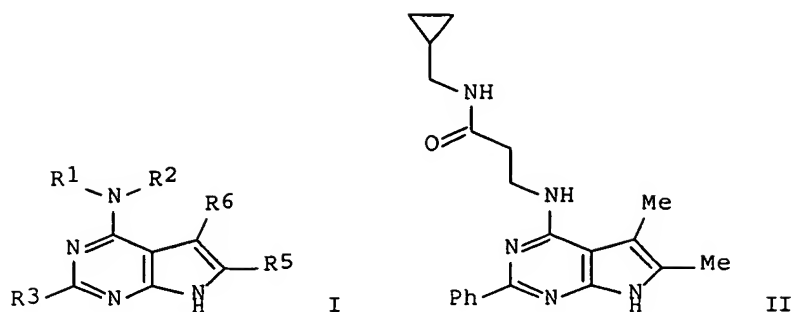
PATENT ASSIGNEE(S): OSI Pharmaceuticals, Inc., USA

SOURCE: U.S., 71 pp., Cont.-in-part of Appl. No. PCT/US99/12135.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English



AB The title compds. [I; R1 = H and R2 = cyclopropylmethylaminocarbonylethyl, cis-3-hydroxycyclopentyl, acetamidobutyl, etc.; or NR1R2 = 3-acetamidopiperadino, 3-hydroxypyrrolidino, 3-methoxycarbonylmethylpyrrolidino, etc.; R3 = (un)substituted cycloalkyl, aryl; R5 = H, alkyl, aryl; R6 = H, alkyl, cycloalkyl] which specifically inhibit the adenosine A3 receptor and are useful for treating a disease associated with A3 adenosine receptor, were prepared. Thus, 4-chloro-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine was reacted with 4-trans-hydroxycyclohexylamine in DMSO at 130°C for 5 h to yield I [R1 = H; R2 = trans-4-hydroxycyclohexyl; R3 = Ph; R5, R6 = Me] in 75% yield after purification which showed  $K_i$  of 13.9 nM against adenosine receptor A1 binding. Some of the compds. I such as II exhibited at least 10 times more selective binding to adenosine receptor A3 than other receptor subtype. Claimed uses of I includes administration of a systemic formulation (i.e. ophthalmic) for the treatment of a disease associated with A3 adenosine receptors in a subject.

IC ICM C07D487-04

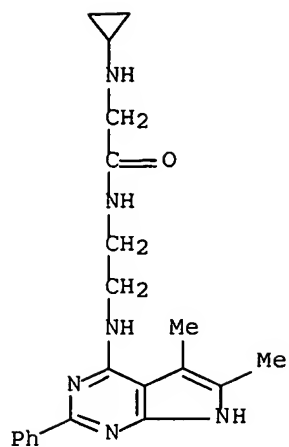
ICS A61K031-519; A61P011-06

INCL 514264100; 544280000

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

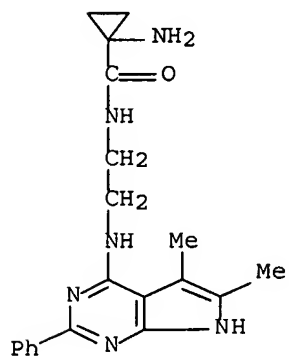
Section cross-reference(s): 1, 63

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	251945-98-9P	251945-99-0P	251946-00-6P	251946-01-7P	251946-02-8P
	251946-03-9P	251946-04-0P	251946-05-1P	251946-06-2P	251946-07-3P
	251946-08-4P	251946-09-5P	251946-10-8P	251946-11-9P	251946-12-0P
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	343631-96-9P	343631-97-0P	343631-98-1P	343631-99-2P	
	343632-00-8P	343632-03-1P	343632-04-2P	343632-05-3P	343632-06-4P
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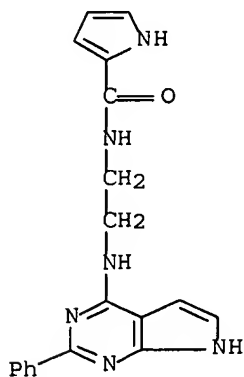
RN 343632-15-5 HCAPLUS

CN Cyclopropanecarboxamide, 1-amino-N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl] - (9CI) (CA INDEX NAME)



RN 343632-38-2 HCAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[2-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl] - (9CI) (CA INDEX NAME)



cycloalkyl of 3-8 C atoms, or arylalkyl having 1-8 C atoms in the alkyl moiety; R3 is H, nitro, halogen, or -NR10R11. R5 is H; alkyl of 1-8 C atoms; alkenyl of 2-7 C atoms; arylalkyl having 1-8 C atoms in the alkyl moiety; alkyl of 1-8 C atoms, substituted with 1-4 substituents selected from -OR7 and halogen; -(CH2)qCR12R13(CH2)rR7; aryl of 6-10 C atoms, optionally mono, di, or trisubstituted with a substituent selected from halogen, cyano, nitro, trifluoromethyl, alkyl of 1-8 carbons optionally substituted with 1-4 substituents selected from OR7 or halogen, cycloalkyl of 3-8 C atoms, aryl of 6-10 C atoms, -NHCONR7R8, and -CO2R7; or a 5-6 membered heterocyclic ring containing 1 to 4 heteroatoms selected from O, S, and N, which is optionally mono- or disubstituted with halogen, alkyl of 1-8 C atoms, or arylalkyl having 1-8 C atoms in the alkyl moiety. R6 is H, alkyl of 1-8 C atoms, alkenyl of 2-7 C atoms, or arylalkyl having 1-8 C atoms in the alkyl moiety; R10 and R11 are each, independently, H, alkyl of 1-8 C atoms, arylalkyl having 1-8 C atoms in the alkyl moiety, -COR7, or -CONR7R8; R12 and R13 are each, independently, H, alkyl of 1-8 C atoms, or aryl of 6-10 C atoms which is optionally substituted with alkyl of 1-8 C atoms or halogen; or R12 and R13 are taken together to form a spiro fused cycloalkyl ring of 3-8 C atoms. M = 0-2; q = 0-5; r = 0-5; s = 1-4; u = 1-4; v = 0-2. Methods of preparation are claimed, comprising (a) reacting A-U-substituted oxirane or a protected form thereof in which a reactive substituent group is protected, with H2NCH2CH2VC6H4W-p or a protected form thereof in which a reactive substituent group is protected; and if required removing any protecting group to give 1. (b) reacting ACH(OPr)CH2I, wherein Pr is a protecting group, with H2NCH2CH2VC6H4W-p or a protected form thereof in which a reactive substituent group is protected; and if required removing any protecting group to give 1 wherein U represents a bond. (c) removing any protecting group from 1 in which at least one substituent carries a protecting group to give 1; or (d) converting a basic compound 1 to a salt thereof by reaction with a pharmaceutically acceptable acid or (e) converting 1 having one or more reactive substituent groups to a different 1; or (f) isolating an isomer of 1 from a mixture thereof.

IC ICM C07D213-74

ICS C07D213-75; C07D471-14; A61K031-44; C07D471-14; C07D235-00; C07D221-00

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 27, 63

IT 108534-48-1P, (4-tert-Butyldiphenylsilyloxy)phenol 122797-04-0P,  
 (2S)-2-[(4-Benzyloxyphenoxy)methyl]oxirane 132059-11-1P,  
 2-Nitro-6-((2S)-oxiranylmethoxy)aniline 197774-51-9P,  
 4-((2S)-Oxiranylmethoxy)-1,3-dihydro-2H-benzimidazol-2-one 391674-00-3P,  
 tert-Butyl(4-oxiranylmethoxyphenoxy)diphenylsilane 391674-01-4P,  
 (4-Benzyloxyphenoxy)tert-butyldiphenylsilane 391674-03-6P, tert-Butyl  
 4-[(3-nitro-2-pyridinyl)amino]phenethylcarbamate 391674-04-7P,  
 N-[4-(2-Aminoethyl)phenyl]-3-nitro-2-pyridinamine 391674-05-8P,  
 (2S)-1-[4-[(tert-Butyldiphenylsilyl)oxy]phenoxy]-3-[[4-[(3-nitro-2-  
 pyridinyl)amino]phenethyl]amino]-2-propanol 391674-09-2P, tert-Butyl  
 4-[(3-amino-2-pyridinyl)amino]phenethylcarbamate 391674-10-5P,  
 tert-Butyl 4-[[3-[[[hexylamino]carbonyl]amino]-2-  
 pyridinyl]amino]phenethylcarbamate 391674-11-6P, N-[2-[4-[2-[[[(2S)-3-[4-  
 [(tert-Butyldiphenylsilyl)oxy]phenoxy]-2-hydroxypropyl]amino]ethyl]anilino  
 ]-3-pyridinyl]-N'-hexylurea 391674-13-8P, tert-Butyl  
 4-[[3-(benzoylamino)-2-pyridinyl]amino]phenethylcarbamate  
 391674-14-9P, N-[2-[4-(2-Aminoethyl)anilino]-3-pyridinyl]benzamide  
 391674-15-0P, N-[2-[4-[2-[[[(2S)-3-[4-[(tert-  
 Butyldiphenylsilyl)oxy]phenoxy]-2-hydroxypropyl]amino]ethyl]anilino]-3-  
 pyridinyl]benzamide 391674-17-2P, tert-Butyl 4-(1-isopropenyl-2-oxo-1,2-  
 dihydro-3H-imidazo[4,5-b]pyridin-3-yl)phenethylcarbamate 391674-19-4P,  
 3-[4-(2-Aminoethyl)phenyl]-1-isopropenyl-1,3-dihydro-2H-imidazo[4,5-  
 b]pyridin-2-one formate 391674-20-7P, 3-[4-[2-[[[(2S)-3-[4-[(tert-  
 Butyldiphenylsilyl)oxy]phenoxy]-2-hydroxypropyl]amino]ethyl]phenyl]-1-

3-[4-[2-[(2S)-2-Hydroxy-3-(4-hydroxyphenoxy)propylamino]ethyl]phenyl]-1-isopropenyl-1,3-dihydroimidazo[4,5-b]pyridin-2-one 391674-21-8P,  
 4-[(2S)-3-[2-[4-[2-(4-Ethylphenyl)imidazo[4,5-b]pyridin-3-yl]phenyl]ethylamino]-2-hydroxypropoxy]phenol hydrochloride 391674-26-3P, 4-[(2S)-2-Hydroxy-3-[2-[4-(2-pentylimidazo[4,5-b]pyridin-3-yl)phenyl]ethylamino]propoxy]phenol 391674-29-6P, 4-[(2S)-3-[2-[4-[2-(4-Cyclohexylphenyl)imidazo[4,5-b]pyridin-3-yl]phenyl]ethylamino]-2-hydroxypropoxy]phenol 391674-33-2P, 4-[(2S)-3-[2-[4-[2-(2-Cyclopentylethyl)imidazo[4,5-b]pyridin-3-yl]phenyl]ethylamino]-2-hydroxypropoxy]phenol 391674-37-6P, 4-[3-[2-[4-[2-(2-Cyclopentylethyl)imidazo[4,5-b]pyridin-3-yl]phenyl]ethylamino]-2-hydroxypropoxy]-1,3-dihydrobenzoimidazol-2-one monohydrochloride 391674-38-7P, 4-[(2S)-2-Hydroxy-3-[2-[4-(2-pentylimidazo[4,5-b]pyridin-3-yl)phenyl]ethylamino]propoxy]-1,3-dihydrobenzoimidazol-2-one 391674-39-8P, 4-[3-[2-[4-[2-[2-Chloro-4-(3-methylpyrazol-1-yl)phenyl]imidazo[4,5-b]pyridin-3-yl]phenyl]ethylamino]-2-hydroxypropoxy]phenol monohydrochloride 391674-50-3P,  
 N-Hexyl-N'-[4-[3-[4-[2-[(2S)-2-hydroxy-3-(4-hydroxyphenoxy)propyl]amino]ethyl]phenyl]-3H-imidazo[4,5-b]pyridin-2-yl]phenyl]urea monohydrochloride 391674-51-4P, 1-Hexyl-3-[3-[4-[2-[(2S)-2-hydroxy-3-(4-hydroxyphenoxy)propylamino]ethyl]phenyl]-3H-imidazo[4,5-b]pyridin-2-yl]phenyl]urea 391674-59-2P, 1-Hexyl-3-[4-[2-[3-[4-[2-[(2S)-2-hydroxy-3-(4-hydroxyphenoxy)propylamino]ethyl]phenyl]-3H-imidazo[4,5-b]pyridin-2-yl]ethyl]phenyl]urea 391674-65-0P, 1-Hexyl-3-[4-[3-[4-[2-[(2S)-2-hydroxy-3-(4-hydroxyphenoxy)propylamino]ethyl]phenyl]-3H-imidazo[4,5-b]pyridin-2-yl]phenyl]urea 391674-66-1P, 4-[(2S)-3-[2-[4-(3-Aminopyridin-2-yloxy)phenyl]ethylamino]-2-hydroxypropoxy]phenol 391674-67-2P, 1-Hexyl-3-[2-[4-[2-[(2S)-2-hydroxy-3-(4-hydroxyphenoxy)propylamino]ethyl]phenylamino]pyridin-3-yl]urea 391674-68-3P, 4-[3-[2-[4-[2-(2-Cyclopentylethyl)imidazo[4,5-b]pyridin-3-yl]phenyl]ethylamino]-2-hydroxypropoxy]-1,3-dihydrobenzoimidazol-2-one 391674-69-4P, N-[2-[4-[2-[(2S)-2-Hydroxy-3-(4-hydroxyphenoxy)propylamino]ethyl]phenylamino]pyridin-3-yl]benzamide 391674-70-7P, 4-[(2S)-3-[2-[4-[2-(4-Ethylphenyl)imidazo[4,5-b]pyridin-3-yl]phenyl]ethylamino]-2-hydroxypropoxy]phenol  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heterocyclic amino alc. beta-3 adrenergic receptor agonists)

IT 391674-13-8P, tert-Butyl 4-[[3-(benzoylamino)-2-pyridinyl]amino]phenethylcarbamate 391674-14-9P, N-[2-[4-(2-Aminoethyl)anilino]-3-pyridinyl]benzamide 391674-15-0P, N-[2-[4-[2-[[[(2S)-3-[4-[(tert-Butyldiphenylsilyl)oxy]phenoxy]-2-hydroxypropyl]amino]ethyl]anilino]-3-pyridinyl]benzamide  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of heterocyclic amino alc. beta-3 adrenergic receptor agonists)

RN 391674-13-8 HCAPLUS

CN Carbamic acid, [2-[4-[[3-(benzoylamino)-2-pyridinyl]amino]phenyl]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



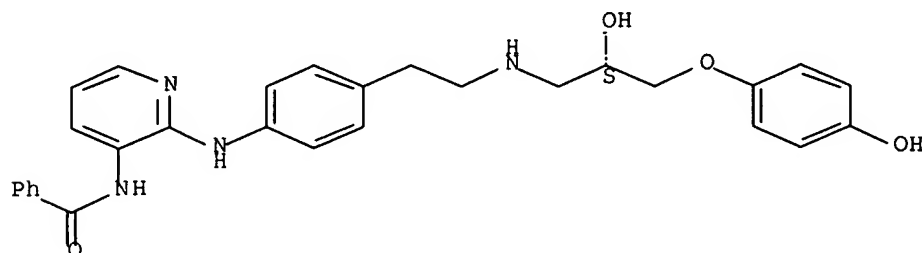
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heterocyclic amino alc. beta-3 adrenergic receptor agonists)

RN 391674-12-7 HCAPLUS

CN Benzamide, N-[2-[[4-[2-[[[(2S)-2-hydroxy-3-(4-hydroxyphenoxy)propyl]amino]ethyl]phenyl]amino]-3-pyridinyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

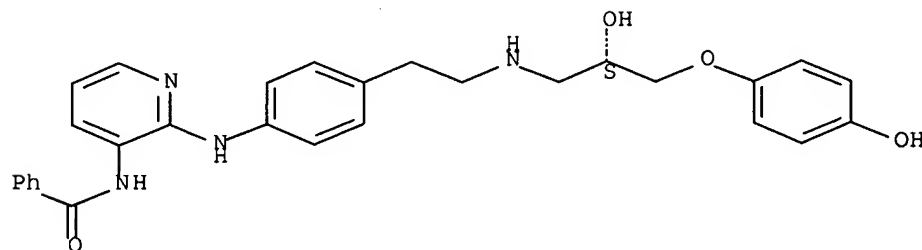


● HCl

RN 391674-69-4 HCAPLUS

CN Benzamide, N-[2-[[4-[2-[[[(2S)-2-hydroxy-3-(4-hydroxyphenoxy)propyl]amino]ethyl]phenyl]amino]-3-pyridinyl]- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L167 ANSWER 4 OF 21 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:713304 HCAPLUS Full-text

DOCUMENT NUMBER: 135:257472

TITLE: Preparation of peptidomimetic ligands for cellular receptors and ion channels

INVENTOR(S): Persons, Paul E.; Holland, Joanne M.; Hauske, James R.

PATENT ASSIGNEE(S): Sepracor, Inc., USA

SOURCE: PCT Int. Appl., 109 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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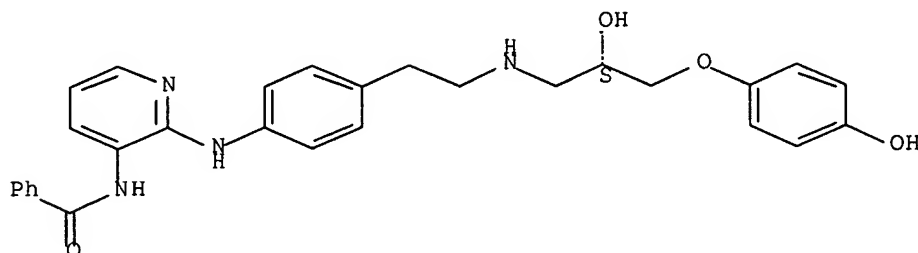
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heterocyclic amino alc. beta-3 adrenergic receptor agonists)

RN 391674-12-7 HCAPLUS

CN Benzamide, N-[2-[[4-[2-[[[(2S)-2-hydroxy-3-(4-hydroxyphenoxy)propyl]amino]ethyl]phenyl]amino]-3-pyridinyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

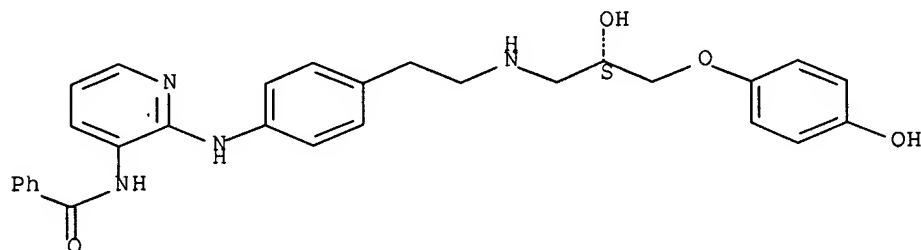


● HCl

RN 391674-69-4 HCAPLUS

CN Benzamide, N-[2-[[4-[2-[[[(2S)-2-hydroxy-3-(4-hydroxyphenoxy)propyl]amino]ethyl]phenyl]amino]-3-pyridinyl]- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L167 ANSWER 4 OF 21 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:713304 HCAPLUS Full-text

DOCUMENT NUMBER: 135:257472

TITLE: Preparation of peptidomimetic ligands for cellular receptors and ion channels

INVENTOR(S): Persons, Paul E.; Holland, Joanne M.; Hauske, James R.

PATENT ASSIGNEE(S): Sepracor, Inc., USA

SOURCE: PCT Int. Appl., 109 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

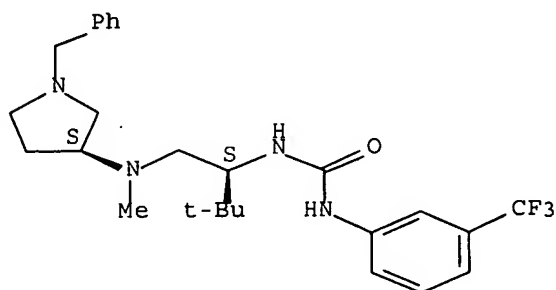
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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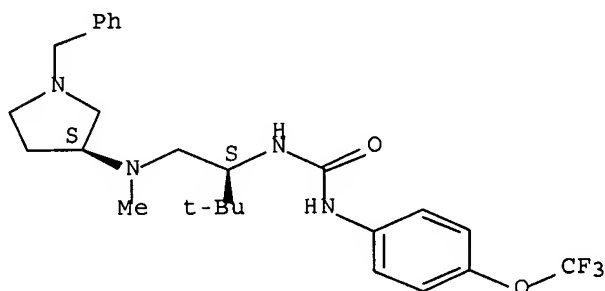
channels)  
 IT 361347-34-4P 361347-38-8P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of peptidomimetic ligands for cellular receptors and ion channels)  
 RN 361347-34-4 HCAPLUS  
 CN Urea, N-[(1S)-2,2-dimethyl-1-[[methyl[(3S)-1-(phenylmethyl)-3-pyrrolidinyl]amino]methyl]propyl]-N'-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 361347-38-8 HCAPLUS  
 CN Urea, N-[(1S)-2,2-dimethyl-1-[[methyl[(3S)-1-(phenylmethyl)-3-pyrrolidinyl]amino]methyl]propyl]-N'-[4-(trifluoromethoxy)phenyl]- (CA INDEX NAME)

Absolute stereochemistry.



L167 ANSWER 5 OF 21 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2001:416773 HCAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 135:46190  
 TITLE: Synthesis and use of substituted pyrrolo[2,3-b]pyrimidines as selective adenosine A1, A2a and A3 receptor antagonists  
 INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan; Witter, David J.  
 PATENT ASSIGNEE(S): Osi Pharmaceuticals, Inc., USA  
 SOURCE: PCT Int. Appl., 368 pp.  
 CODEN: PIXXD2

d]pyrimidine hydrochloride was reacted with D-prolinol (2.3 mol equiv) in DMSO at 120°C for 18 h to yield III in 13% yield after purification. Compound I [R1 = AcNHCH2CH2; R2 = H; R3 = Ph; R4, R5 = Me; II] exhibited selective binding to adenosine receptor A1 with IC50 = 82.8 nM. Compound II also had Ki = 9.8 nM (vs. Ki = 7.1 for control ligand 8-cyclopentyl-1,3-dipropylxanthine (DPCPX)). Pyrimidine III binds 5 times more selectively to adenosine receptor A2a than A1, A2b or A3 (no data). Compound I [R1 = AcNH(CH2)4; R2 = H; R3 = Ph; R4, R5 = Me] is 10 times more selective for A3 than the other receptor subtypes. ClogP (calculated partition coefficient between octanol and H2O) values were determined for selected example compds. Claimed uses of I includes administration of a systemic formulation (i.e. ophthalmic) for the treatment of a disease associated with A1, A2a, and A3 adenosine receptors in a subject.

IC ICM A61K031-519

ICS C07D487-04

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

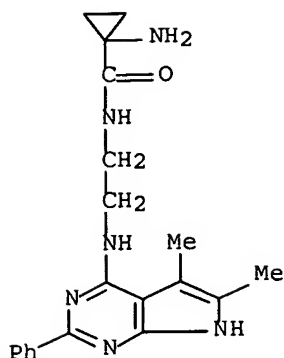
Section cross-reference(s): 1, 63

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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

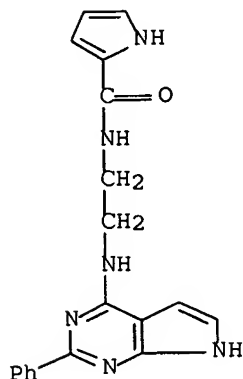
(preparation and use of substituted 7H-pyrrolo[2,3-b]pyrimidines as selective adenosine A1, A2a and A3 receptor antagonists)

IT 251946-27-7P 343631-99-2P 343632-15-5P



RN 343632-38-2 HCAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[2-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L167 ANSWER 6 OF 21 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:331315 HCAPLUS Full-text

DOCUMENT NUMBER: 134:340515

TITLE: Preparation and use of dihydropyrimidines as selective antagonists for human  $\alpha 1A$  receptors

INVENTOR(S): Nagarathnam, Dhanapalan; Wong, Wai C.; Miao, Shou Wu; Gluchowski, Charles; Patane, Michael A.

PATENT ASSIGNEE(S): Synaptic Pharmaceutical Corporation, USA

SOURCE: U.S., 29 pp., Cont.-in-part of Appl. No. PCT/US95/15025.

CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 6228861	B1	20010508	US 1998-68782	19981110 <--

α1A receptors)  
 IT 318237-17-1P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (preparation of dihydropyrimidines as selective antagonists for human α1A receptors)

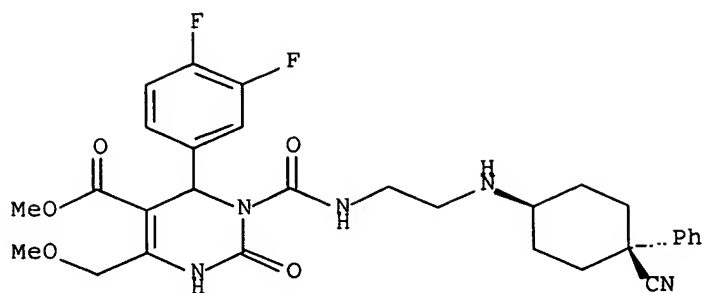
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 318237-26-2P 318237-27-3P 318237-28-4P  
 338465-41-1P 338465-42-2P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of dihydropyrimidines as selective antagonists for human α1A receptors)

IT 338465-43-3P  
 RL: BYP (Byproduct); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of dihydropyrimidines as selective antagonists for human α1A receptors)

IT 179482-24-7P 179482-25-8P 179482-26-9P 179482-45-2P 179482-46-3P  
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 318237-16-0P 338465-44-4P 338465-45-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of dihydropyrimidines as selective antagonists for human α1A receptors)

IT 191353-50-1P 191353-51-2P 191353-52-3P  
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 318236-87-2P 318236-88-3P  
 RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of dihydropyrimidines as selective antagonists for human α1A receptors)

RN 191353-50-1 HCAPLUS  
 CN 1(2H)-Pyrimidinecarboxamide, 5-acetyl-N-[2-[(cis-4-cyano-4-phenylcyclohexyl)amino]ethyl]-3,6-dihydro-4-(methoxymethyl)-2-oxo-6-(3,4,5-

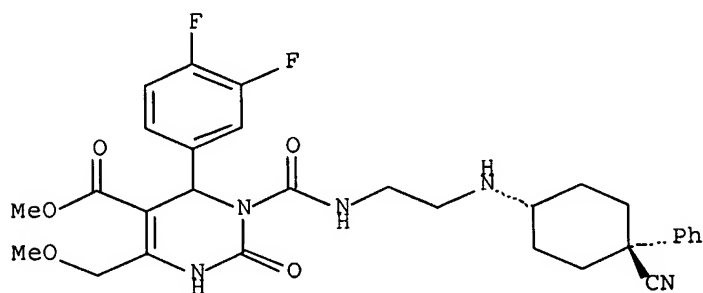


● HCl

RN 191353-53-4 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[(trans-4-cyano-4-phenylcyclohexyl)amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, monohydrochloride, (+)-(9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

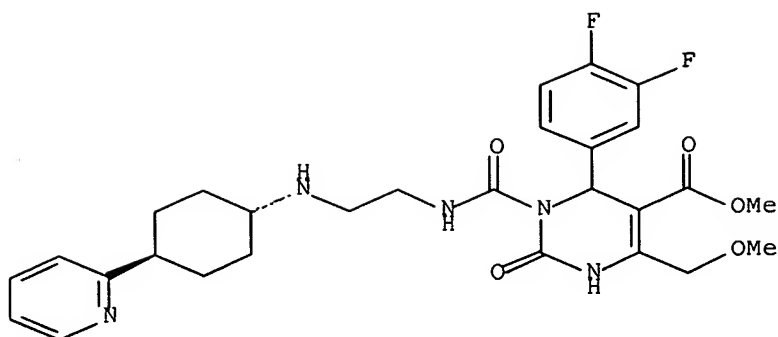


● HCl

RN 191353-59-0 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-1-[[[2-[[cis-4-(methoxycarbonyl)-4-phenylcyclohexyl]amino]ethyl]amino]carbonyl]-4-(methoxymethyl)-2-oxo-, methyl ester, monohydrochloride, (+)-(9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

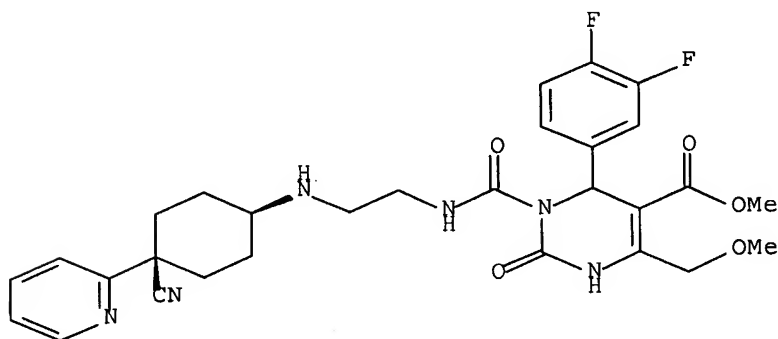


●2 HCl

RN 318236-88-3 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[cis-4-cyano-4-(2-pyridinyl)cyclohexyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, dihydrochloride, (+)-(9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



●2 HCl

IT 318237-17-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of dihydropyrimidines as selective antagonists for human  $\alpha_1A$  receptors)

RN 318237-17-1 HCAPLUS

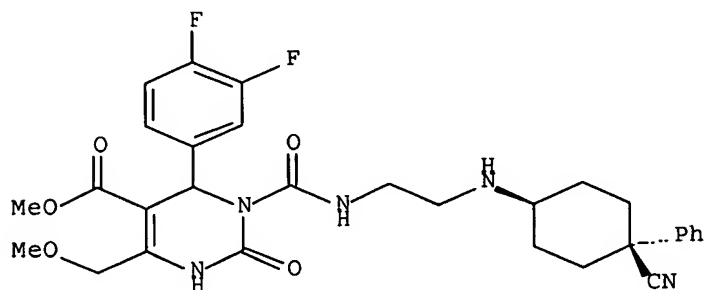
CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-1-[[[2-[(trans-4-phenylcyclohexyl)amino]ethyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

Relative stereochemistry.



phenylcyclohexyl) amino] ethyl] amino] carbonyl] -6- (3,4-difluorophenyl) -  
1,2,3,6-tetrahydro-4- (methoxymethyl)-2-oxo-, methyl ester,  
monohydrochloride, (-)- (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.

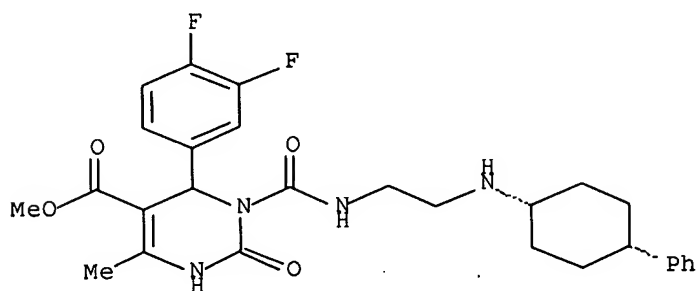


● HCl

RN 191353-56-7 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6- (3,4-difluorophenyl) -1,2,3,6-tetrahydro-4-  
methyl-2-oxo-1-[[[2-[(cis-4-phenylcyclohexyl) amino] ethyl] amino] carbonyl] -,  
methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.



● HCl

RN 191353-57-8 HCAPLUS

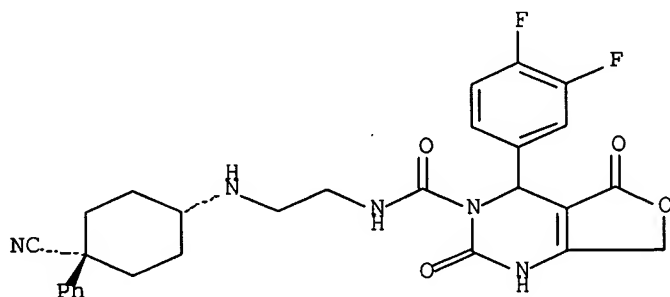
CN 5-Pyrimidinecarboxylic acid, 6- (3,4-difluorophenyl) -1,2,3,6-tetrahydro-4-  
methyl-2-oxo-1-[[[2-[(trans-4-phenylcyclohexyl) amino] ethyl] amino] carbonyl] -  
, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 191353-67-0 HCAPLUS

CN Furo[3,4-d]pyrimidine-3(4H)-carboxamide, N-[2-[(cis-4-cyano-4-phenylcyclohexyl)amino]ethyl]-4-(3,4-difluorophenyl)-1,2,5,7-tetrahydro-2,5-dioxo-, monohydrochloride, (+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

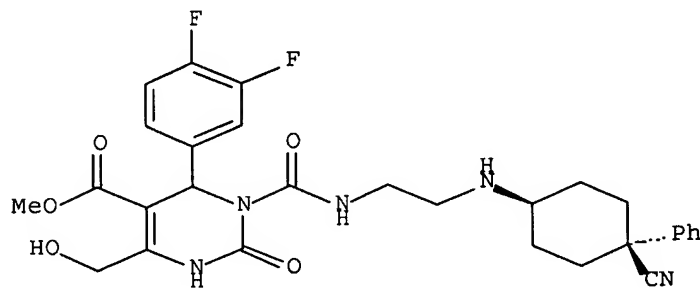


● HCl

RN 191353-71-6 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[(cis-4-cyano-4-phenylcyclohexyl)amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(hydroxymethyl)-2-oxo-, methyl ester, (+)- (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

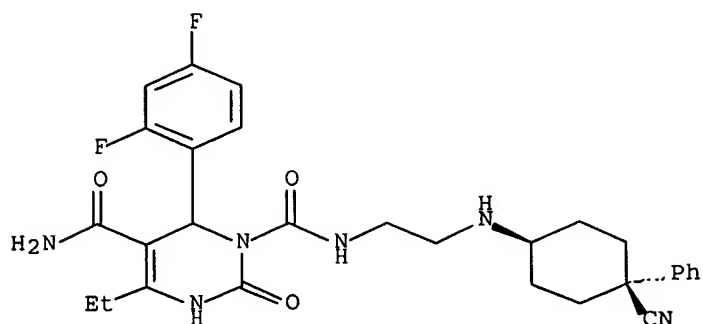


RN 191353-72-7 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[(cis-4-cyano-4-phenylcyclohexyl)amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, (+)- (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

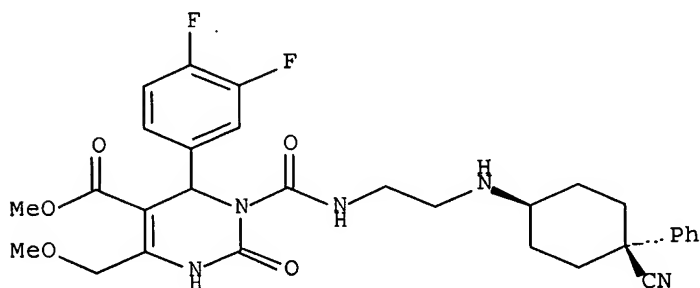
Rotation (+). Absolute stereochemistry unknown.



RN 318236-93-0 HCAPLUS

516238-93-0 NCM 100  
CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[(cis-4-cyano-4-phenylcyclohexyl)amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (+)- (CA INDEX NAME)

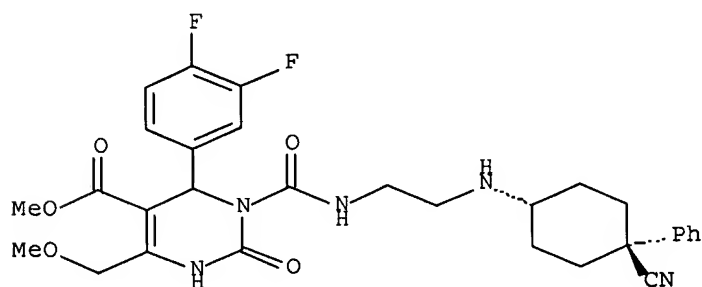
Rotation (+). Absolute stereochemistry unknown.

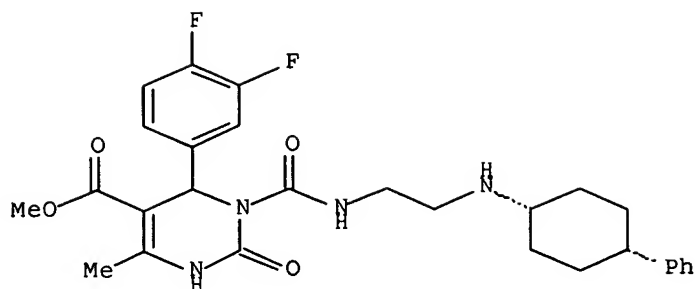


RN 318236-94-1 HCAPLUS

5-Pyrimidinecarboxylic acid, 1-[[[2-[(trans-4-cyano-4-phenylcyclohexyl)amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (+)- (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

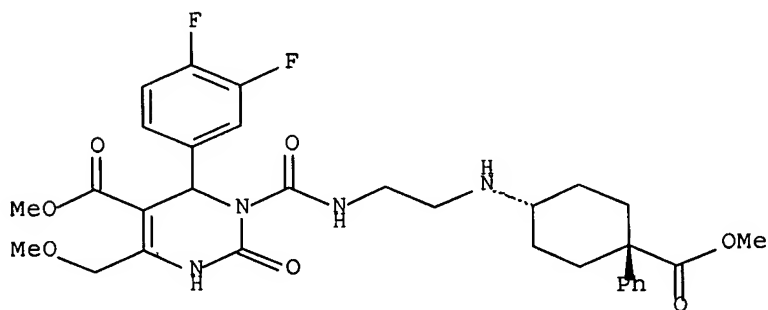




RN 318236-98-5 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-1-[[[2-[[cis-4-(methoxycarbonyl)-4-phenylcyclohexyl]amino]ethyl]amino]carbonyl]-4-(methoxymethyl)-2-oxo-, methyl ester, (+)- (CA INDEX NAME)

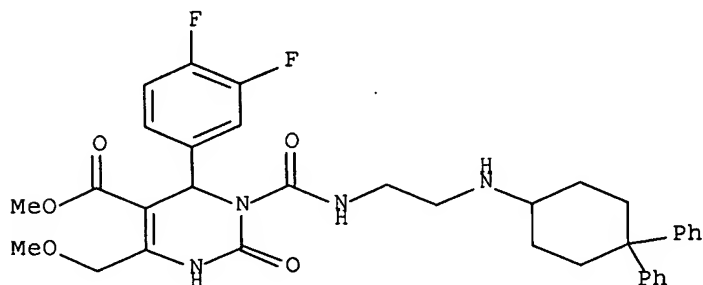
Rotation (+). Absolute stereochemistry unknown.



RN 318236-99-6 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1-[[[2-[[4,4-diphenylcyclohexyl]amino]ethyl]amino]carbonyl]-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (+)- (CA INDEX NAME)

Rotation (+).



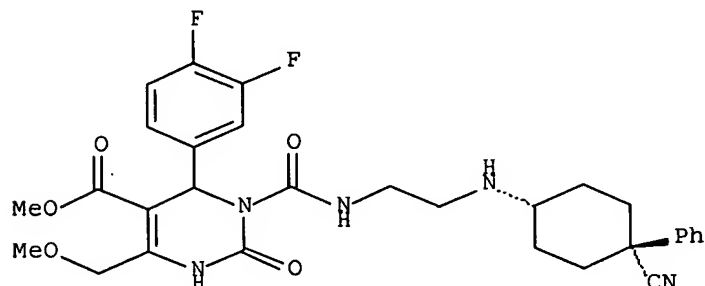
RN 318237-00-2 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[cis-4-cyano-4-(2-fluorophenyl)cyclohexyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-, methyl ester, (+)- (CA INDEX NAME)

RN 318237-05-7 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[(cis-4-cyano-4-phenylcyclohexyl)amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester (CA INDEX NAME)

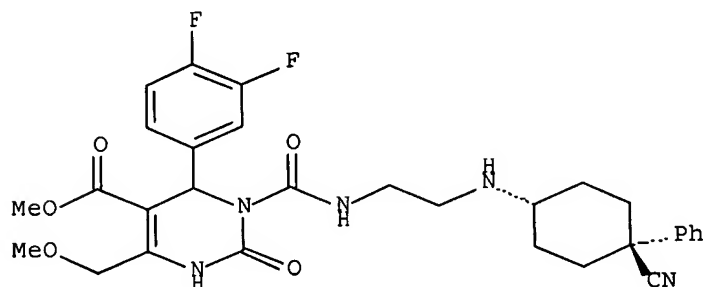
Relative stereochemistry.



RN 318237-07-9 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[(trans-4-cyano-4-phenylcyclohexyl)amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester (CA INDEX NAME)

Relative stereochemistry.



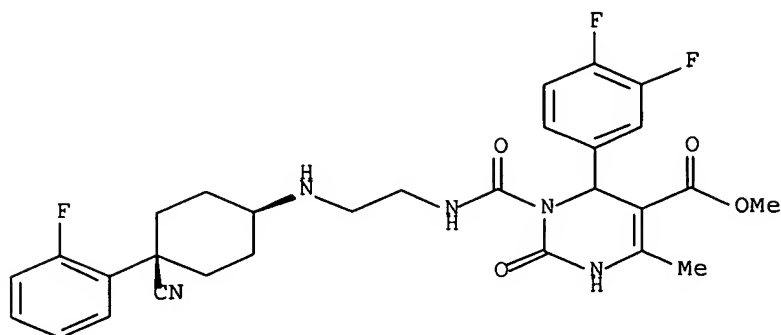
RN 318237-09-1 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[(trans-4-cyano-4-phenylcyclohexyl)amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (-)- (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.

1,2,3,6-tetrahydro-4-methyl-2-oxo-, methyl ester (CA INDEX NAME)

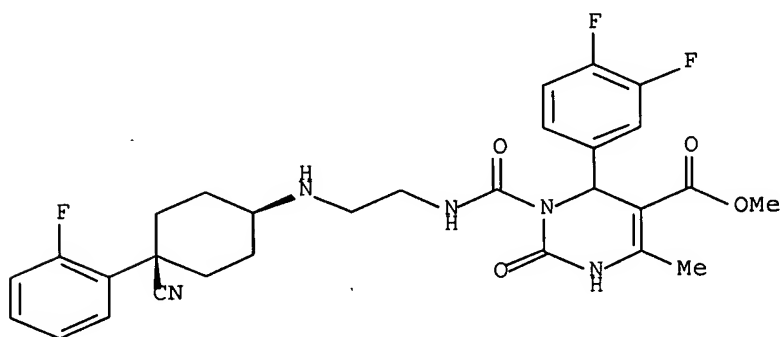
Relative stereochemistry.



RN 318237-19-3 HCAPLUS

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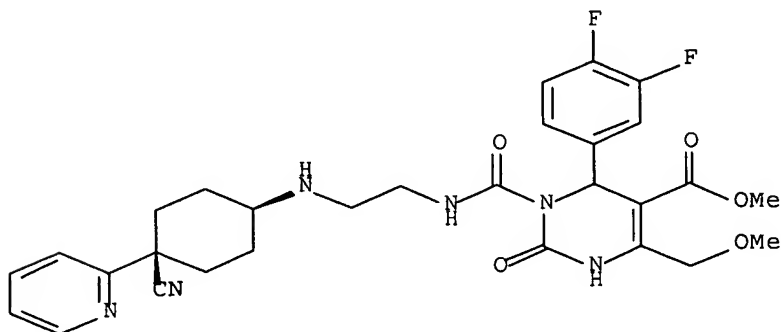
Rotation (-). Absolute stereochemistry unknown.

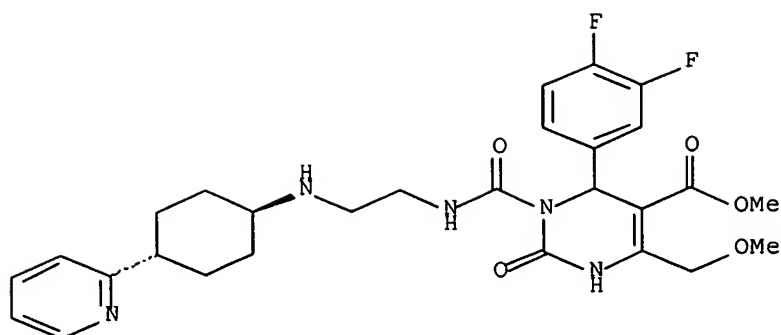


RN 318237-20-6 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[[cis-4-cyano-4-(2-pyridinyl)cyclohexyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester (CA INDEX NAME)

Relative stereochemistry.

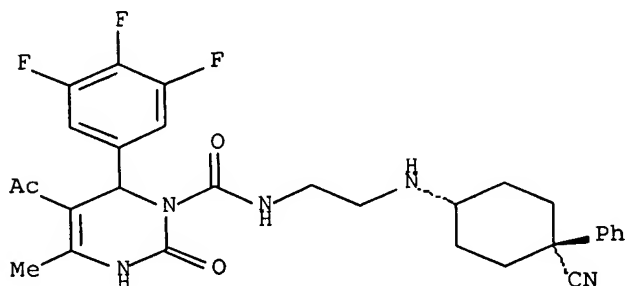




RN 318237-24-0 HCAPLUS

CN 1(2H)-Pyrimidinecarboxamide, 5-acetyl-N-[2-[(cis-4-cyano-4-phenylcyclohexyl)amino]ethyl]-3,6-dihydro-4-methyl-2-oxo-6-(3,4,5-trifluorophenyl)- (CA INDEX NAME)

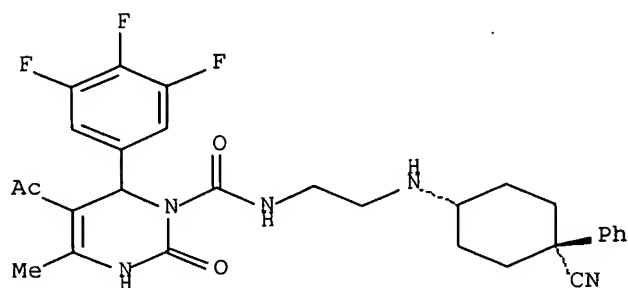
Relative stereochemistry.



RN 318237-25-1 HCAPLUS

CN 1(2H)-Pyrimidinecarboxamide, 5-acetyl-N-[2-[(cis-4-cyano-4-phenylcyclohexyl)amino]ethyl]-3,6-dihydro-4-methyl-2-oxo-6-(3,4,5-trifluorophenyl)-, (+)- (CA INDEX NAME)

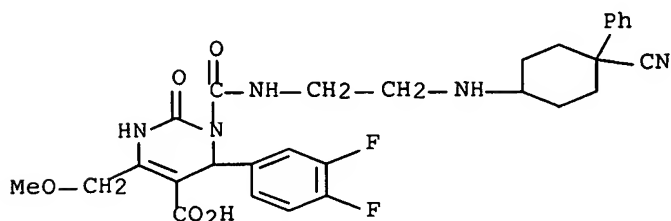
Rotation (+). Absolute stereochemistry unknown.



RN 318237-26-2 HCAPLUS

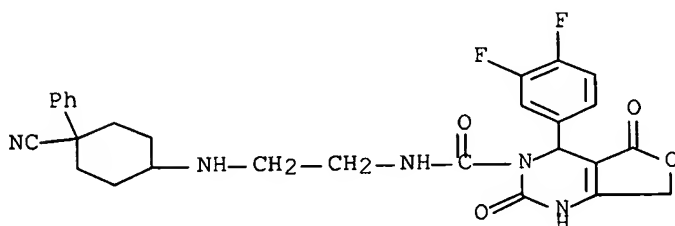
CN 1(2H)-Pyrimidinecarboxamide, 5-acetyl-N-[2-[(cis-4-cyano-4-phenylcyclohexyl)amino]ethyl]-3,6-dihydro-4-methyl-2-oxo-6-(3,4,5-trifluorophenyl)-, (-)- (CA INDEX NAME)

phenylcyclohexyl)amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-  
1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo- (CA INDEX NAME)



RN 338465-42-2 HCAPLUS

CN Furo[3,4-d]pyrimidine-3(4H)-carboxamide, N-[2-[(4-cyano-4-phenylcyclohexyl)amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,5,7-tetrahydro-2,5-dioxo- (CA INDEX NAME)



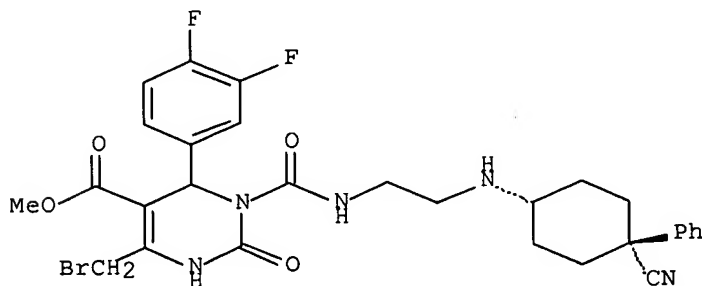
IT 338465-43-3P

RL: BYP (Byproduct); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of dihydropyrimidines as selective antagonists for human  $\alpha_1A$  receptors)

RN 338465-43-3 HCAPLUS

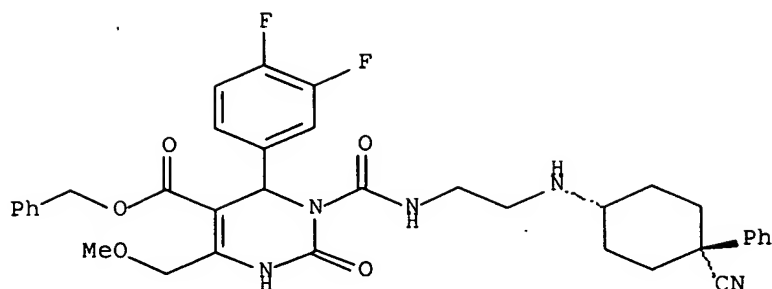
CN 5-Pyrimidinecarboxylic acid, 4-(bromomethyl)-1-[[[2-[(cis-4-cyano-4-phenylcyclohexyl)amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-2-oxo-, methyl ester, monohydrochloride, (+)-(9CI)  
(CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



● HCl





REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L167 ANSWER 7 OF 21 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:88189 HCAPLUS Full-text

DOCUMENT NUMBER: 134:280817

TITLE: Synthesis of tricyclic triazepinones related to nevirapine

AUTHOR(S): Castellano, Sabrina; Stefancich, Giorgio; La Colla, Paolo; Musiu, Chiara

CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Universita di Trieste, Trieste, 1-34127, Italy

SOURCE: Journal of Heterocyclic Chemistry (2000), 37(6), 1539-1542

CODEN: JHTCAD; ISSN: 0022-152X

PUBLISHER: HeteroCorporation

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:280817

AB Two novel tricyclic triazepinones, 5,10-dihydro-5-ethyl-11H-pyrrolo[1,2-b][1,2,5]benzotriazepin-11-one 5 and 5,11-dihydro-11-ethyl-6H-pyrido[3,2-f]pyrrolo[1,2-b][1,2,5]triazepin-6-one 6, structurally related to the reverse transcriptase inhibitor nevirapine were prepared from N-(2-nitrophenyl)- and N-(3-nitro-2-pyridinyl)-1H-pyrrol-1-amine 7a, b. The synthetic sequence includes ethylation with EtBr, reduction of the nitro group, triphosgene reaction followed by intramol. cyclization. Activity of the two compds. against the HIV-1 multiplication in acutely infected cells is also reported, with 5 (EC50 = 48 µM) being more potent than 6 (EC50 >200 µM), but less so than nevirapine itself (EC50 = 0.1 µM).

CC 28-22 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1

IT 332379-59-6P 332379-61-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and thermal cyclization of)

IT 332379-61-0P

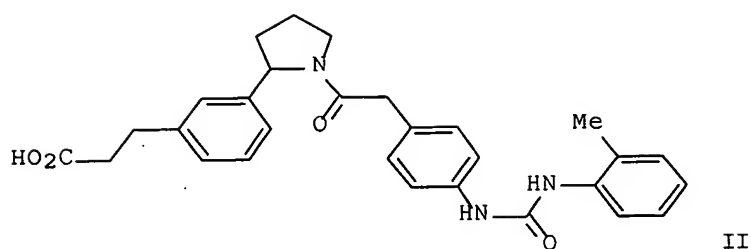
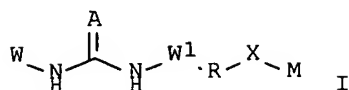
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and thermal cyclization of)

RN 332379-61-0 HCAPLUS

CN Urea, N,N'-bis[2-(ethyl-1H-pyrrol-1-ylamino)-3-pyridinyl]- (CA INDEX NAME)

US 1999-141602P	P 19990630 <--
US 1999-141692P	P 19990630 <--
WO 2000-US18079	W 20000630 <--
US 2001-34585	A3 20011228
US 2004-787905	A3 20040226

OTHER SOURCE(S) : MARPAT 134:86149  
GI



AB The title compds. [I; W = (un)substituted aryl, heteroaryl; W1 = (un)substituted arylene, heteroarylene; A = O, S, NH; R = a bond, alkenylene, (CH<sub>2</sub>)<sub>n</sub>; n = 1-2; X = CO, CH<sub>2</sub>, SO<sub>2</sub>; M = substituted pyrrolidinyl, thiazolidinyl, etc.] which selectively inhibit the binding of ligands to α<sub>4</sub>β<sub>1</sub> integrin (VLA-4), and therefore are useful in the treatment of conditions associated with VLA-4 mediated cell adhesion, including, but not limited to, such conditions as inflammatory and autoimmune responses, diabetes, asthma, psoriasis, inflammatory bowel disease, transplantation rejection, and tumor metastasis, were prepared E.g., a multi-step synthesis of the urea II which showed K<sub>i</sub> of < 50 nM against VLA-4 receptors binding, was given.

IC ICM A61K031-40

ICS A61K031-4025; C07D207-12; C07D207-14; C07D401-12; C07D403-12

CC 27-10 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1

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RL: BAC (Biological activity or effector, except adverse); BSU  
(Biological study, unclassified); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(preparation of di-Ph ureas as VLA-4 inhibitors)

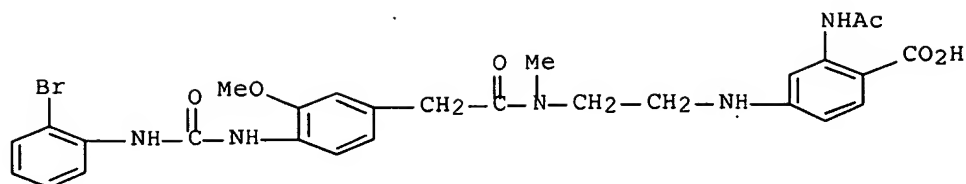
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

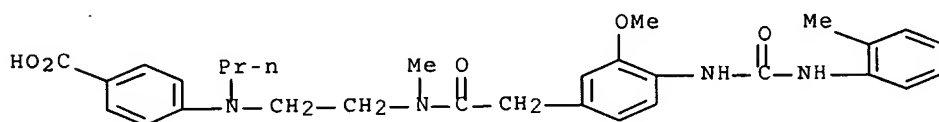
(preparation of di-Ph ureas as VLA-4 inhibitors)

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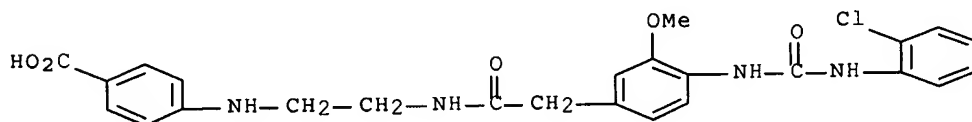
RN 317362-82-6 HCAPLUS

CN Benzoic acid, 4-[[2-[[[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]acetyl]methylamino]ethyl]propylamino]- (9CI) (CA INDEX NAME)



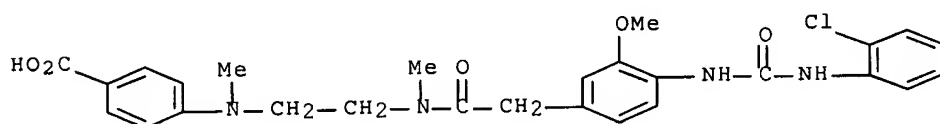
RN 317362-85-9 HCAPLUS

CN Benzoic acid, 4-[[2-[[[4-[[[(2-chlorophenyl)amino]carbonyl]amino]-3-methoxyphenyl]acetyl]amino]ethyl]amino]- (9CI) (CA INDEX NAME)



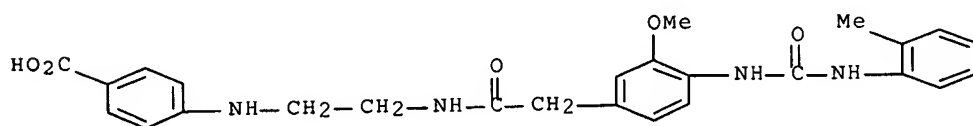
RN 317362-86-0 HCAPLUS

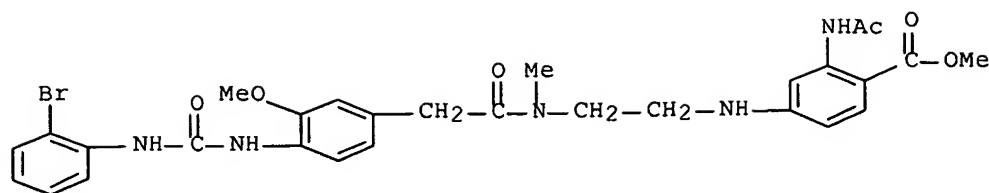
CN Benzoic acid, 4-[[2-[[[4-[[[(2-chlorophenyl)amino]carbonyl]amino]-3-methoxyphenyl]acetyl]methylamino]ethyl]methylamino]- (9CI) (CA INDEX NAME)



RN 317362-92-8 HCAPLUS

CN Benzoic acid, 4-[[2-[[[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]acetyl]amino]ethyl]amino]- (9CI) (CA INDEX NAME)

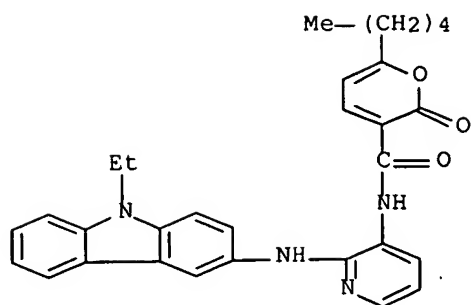




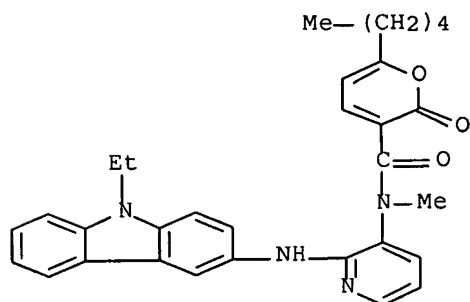
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L167 ANSWER 9 OF 21 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2000:117043 HCAPLUS Full-text  
 DOCUMENT NUMBER: 132:151680  
 TITLE: Preparation of carbazoles, isoquinolines, indoles, and related compounds as follicle stimulating hormone mimetics for the treatment of infertility.  
 INVENTOR(S): El Tayer, Nabil; Reddy, Adulla; Buckler, David; Magar, Sharad  
 PATENT ASSIGNEE(S): Applied Research Systems Ars Holding N. V., Neth. Antilles  
 SOURCE: PCT Int. Appl., 62 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

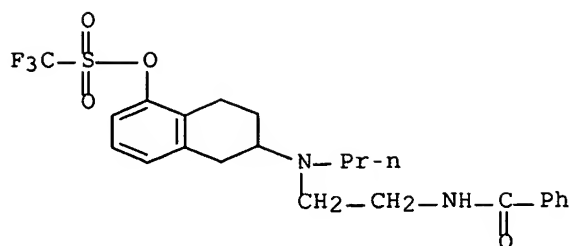
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000008015	A2	20000217	WO 1999-US17755	19990805 <--
WO 2000008015	A3	20000511		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2339018	A1	20000217	CA 1999-2339018	19990805 <--
AU 9953931	A	20000228	AU 1999-53931	19990805 <--
AU 772373	B2	20040422		
US 6235755	B1	20010522	US 1999-369222	19990805 <--
EP 1102763	A2	20010530	EP 1999-939686	19990805 <--
EP 1102763	B1	20041013		
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JP 2002522433	T	20020723	JP 2000-563648	19990805 <--
EP 1380582	A1	20040114	EP 2003-23514	19990805 <--
EP 1380582	B1	20060614		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
AT 279407	T	20041015	AT 1999-939686	19990805 <--
PT 1102763	T	20050131	PT 1999-939686	19990805 <--
ES 2228084	T3	20050401	ES 1999-939686	19990805 <--
IL 141063	A	20050619	IL 1999-141063	19990805 <--
AT 329911	T	20060715	AT 2003-23514	19990805 <--



RN 258278-14-7 HCAPLUS  
 CN 2H-Pyran-3-carboxamide, N-[2-[(9-ethyl-9H-carbazol-3-yl)amino]-3-pyridinyl]-N-methyl-2-oxo-6-pentyl- (CA INDEX NAME)

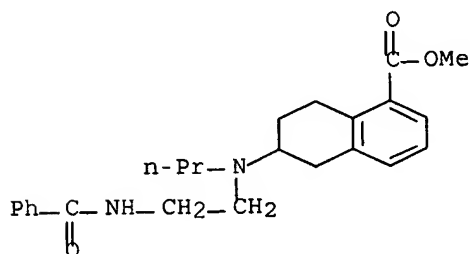


L167 ANSWER 10 OF 21 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2000:9445 HCAPLUS Full-text  
 DOCUMENT NUMBER: 132:131789  
 TITLE: C5-Substituted derivatives of 5-OMe-BPAT: synthesis and interactions with dopamine D2 and serotonin 5-HT1A receptors  
 AUTHOR(S): Homan, Evert J.; Tulp, Martin Th. M.; Nilsson, Jonas E.; Wikstrom, Hakan V.; Grol, Cor J.  
 CORPORATE SOURCE: Department of Medicinal Chemistry, University Centre for Pharmacy, University of Groningen, Groningen, NL-9713 AV, Neth.  
 SOURCE: Bioorganic & Medicinal Chemistry (1999), 7(11), 2541-2548  
 CODEN: BMECEP; ISSN: 0968-0896  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Eight new C5-substituted derivs. of the potential atypical antipsychotic agent 5-methoxy-2-[N-(2-benzamidoethyl)-N-n-propylamino]tetralin (5-OMe-BPAT, I) have been prepared by chemical conversion of the 5-trifluoromethylsulfonyloxy (triflate) analog via various Stille-type cross-couplings, a Heck reaction, and an amidation in moderate to good yields. The 5-acetyl, 5-cyano, 5-Me, 5-(2-furyl), 5-Ph, Me 5-carboxylate, and the 5-carboxamido analogs thus obtained, the previously disclosed 5-methoxy, 5-hydroxy, and 5-unsubstituted analogs, and the 5-triflate analog were evaluated for their ability to compete for [3H]-spiperone binding to rat striatal membranes containing dopamine D2 receptors, and their ability to compete for [3H]-8-OH-DPAT binding to rat



RN 257294-13-6 HCAPLUS

CN 1-Naphthalenecarboxylic acid, 6-[[2-(benzoylamino)ethyl]propylamino]-5,6,7,8-tetrahydro-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

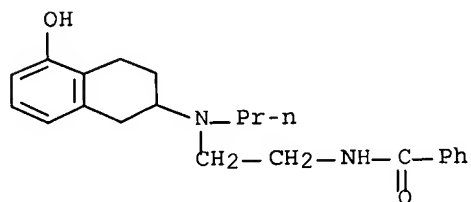
IT 257294-04-5

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)

(preparation and interactions with dopamine D2 and serotonin 5-HT1A receptors of benzamide aminotetralin derivs.)

RN 257294-04-5 HCAPLUS

CN Benzamide, N-[2-[propyl(1,2,3,4-tetrahydro-5-hydroxy-2-naphthalenyl)amino]ethyl]- (CA INDEX NAME)

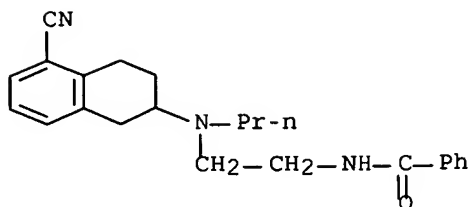


IT 257294-07-8P 257294-08-9P 257294-09-0P  
257294-10-3P 257294-11-4P 257294-12-5P  
257294-14-7P

RL: BAC (Biological activity or effector, except adverse); BSU



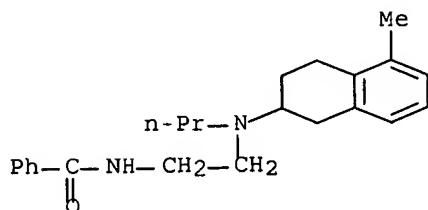
naphthalenyl]propylamino]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 257294-10-3 HCAPLUS

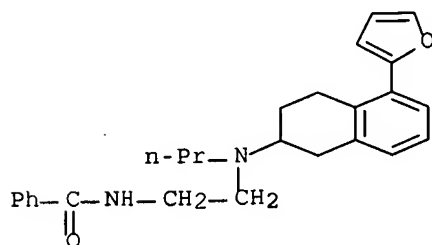
CN Benzamide, N-[2-[propyl(1,2,3,4-tetrahydro-5-methyl-2-naphthalenyl)amino]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 257294-11-4 HCAPLUS

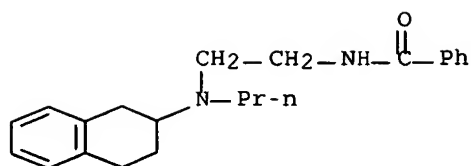
CN Benzamide, N-[2-[[5-(2-furanyl)-1,2,3,4-tetrahydro-2-naphthalenyl]propylamino]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 257294-12-5 HCAPLUS

CN Benzamide, N-[2-[propyl(1,2,3,4-tetrahydro-5-phenyl-2-naphthalenyl)amino]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L167 ANSWER 11 OF 21 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:485957 HCAPLUS Full-text

DOCUMENT NUMBER: 131:243049

TITLE: Synthesis and pharmacology of the enantiomers of the potential atypical antipsychotic agents 5-OMe-BPAT and 5-OMe-(2,6-di-OMe)-BPAT

AUTHOR(S): Homan, Evert J.; Coppinga, Swier; Unelius, Lena; Jackson, David M.; Wikstrom, Hakan V.; Grol, Cor J.

CORPORATE SOURCE: Department of Medicinal Chemistry, University Centre for Pharmacy, University of Groningen, Groningen, NL-9713 AV, Neth.

SOURCE: Bioorganic & Medicinal Chemistry (1999), 7(7), 1263-1271

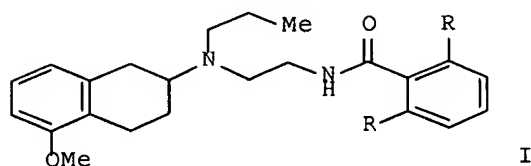
CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

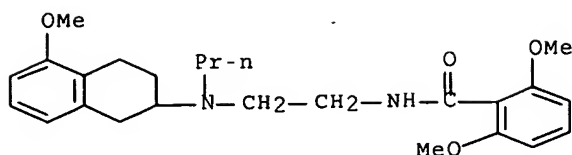
LANGUAGE: English

GI



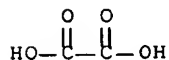
AB The optically pure enantiomers of the potential atypical antipsychotic agents methoxybenzamidoethyl-N-propylaminotetralin I (R = H) (5-MeO-BPAT) and methoxy-N-dimethoxybenzamidoethyl-N-n-propylaminotetralin I (R = MeO) were synthesized and evaluated for their in vitro binding affinities at  $\alpha 1$ -,  $\alpha 2$ -, and  $\beta$ -adrenergic, muscarinic, dopamine D1, D2A, and D3, and serotonin 5-HT1A and 5-HT2 receptors. In addition, their intrinsic efficacies at serotonin 5-HT1A receptors were established in vitro. Both enantiomers of I (R = H) had high affinities for dopamine D2A, D3, and serotonin 5-HT1A receptors, moderate affinities for  $\alpha 1$ -adrenergic and serotonin 5-HT2 receptors, and no affinity ( $K_i > 1000$  nM) for the other receptor subtypes. Both enantiomers of I (R = MeO) had lower affinities for the dopamine D2A and the serotonin 5-HT1A receptor, compared to the enantiomers of I (R = H), and hence showed some selectivity for the dopamine D3 receptor. The interactions with the receptors were stereospecific, since the serotonin 5-HT1A receptor preferred the (S)-enantiomers of I while the dopamine D2A and D3 receptors preferred the (R)-enantiomers of I. The intrinsic efficacies at the serotonin 5-HT1A receptor were established by measuring their ability to inhibit VIP-induced cAMP

CRN 244239-81-4  
CMF C25 H34 N2 O4



CM 2

CRN 144-62-7  
CMF C2 H2 O4



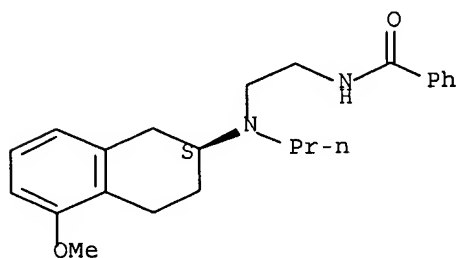
IT 244239-75-6P 244239-76-7P 244239-78-9P  
244239-80-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of propylbenzoylaminotetralins and their enantiomers as  
potential antipsychotic agents and their binding to adrenergic,  
dopamine, and serotonin receptors)

RN 244239-75-6 HCAPLUS

CN Benzamide, N-[2-[propyl[(2S)-1,2,3,4-tetrahydro-5-methoxy-2-naphthalenyl]amino]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

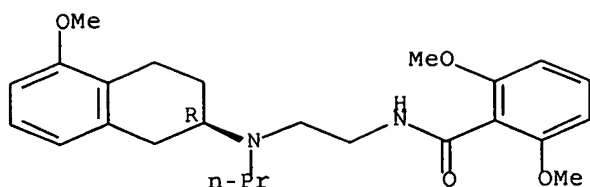


● HCl

RN 244239-76-7 HCAPLUS

CN Benzamide, N-[2-[propyl[(2R)-1,2,3,4-tetrahydro-5-methoxy-2-naphthalenyl]amino]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

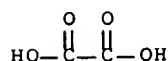
Absolute stereochemistry. Rotation (+).



CM 2

CRN 144-62-7

CMF C2 H2 O4



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L167 ANSWER 12 OF 21 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:460399 HCAPLUS Full-text

DOCUMENT NUMBER: 131:87814

TITLE: Indole derivatives as inhibitors of factor Xa, and their preparation and use as anticoagulants

INVENTOR(S): Defossa, Elisabeth; Heinelt, Uwe; Klingler, Otmar; Zoller, Gerhard; Al-Obeidi, Fahad; Walser, Armin; Wildgoose, Peter; Matter, Hans

PATENT ASSIGNEE(S): Hoechst Marion Roussel Deutschland GmbH, Germany

SOURCE: PCT Int. Appl., 199 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9933800	A1	19990708	WO 1998-EP8030	19981210 <--
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW			
RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
CA 2316172	A1	19990708	CA 1998-2316172	19981210 <--
AU 9920528	A	19990719	AU 1999-20528	19981210 <--
AU 743881	B2	20020207		
BR 9814340	A	20001003	BR 1998-14340	19981210 <--
EP 1042287	A1	20001011	EP 1998-965244	19981210 <--
EP 1042287	B1	20050420		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, FI			

compds. I were prepared For instance, 1H-indole-2-carboxylic acid Et ester underwent a 5-step sequence to give title salt II. This preparation involved (1) N-alkylation with 3-cyanobenzyl bromide, (2) alkaline hydrolysis of the ester, (3) amidation with 4-(Me<sub>2</sub>N)C<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>NH<sub>2</sub>.2HCl, (4) conversion of the nitrile to a thioamide, and (5) quaternization at dimethylamino, and ammonolysis of the thioamide to an amidine. In an assay using human factor Xa in vitro, II had a K<sub>i</sub> value of 0.090 μM.

IC ICM C07D209-42

ICS A61K031-40; C07D401-12; C07D403-10; C07D401-06; C07D471-04;  
C07D471-04; C07D221-00; C07D209-00

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1, 7

IT 229949-99-9P 229950-02-1P 229950-04-3P 229950-07-6P 229950-10-1P  
229950-13-4P 229950-16-7P 229950-19-0P 229950-22-5P 229950-25-8P  
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229953-04-2P 229953-06-4P 229953-08-6P 229953-10-0P  
229953-12-2P 229953-14-4P

RL: BAC (Biological activity or effector, except adverse); BSU  
(Biological study, unclassified); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(target compound; preparation of indole derivs. as inhibitors of factor Xa)

IT 229953-08-6P 229953-10-0P

RL: BAC (Biological activity or effector, except adverse); BSU  
(Biological study, unclassified); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(target compound; preparation of indole derivs. as inhibitors of factor Xa)

RN 229953-08-6 HCAPLUS

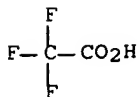
CN 1H-Indole-2-carboxamide, 1-[[3-(aminoiminomethyl)phenyl)methyl]-4-hydroxy-  
N-[2-(methyl-1-naphthalenylamino)ethyl]-, mono(trifluoroacetate) (salt)  
(9CI) (CA INDEX NAME)

CM 1

CM 2

CRN 76-05-1

CMF C2 H F3 O2



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L167 ANSWER 13 OF 21 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:404839 HCAPLUS Full-text

DOCUMENT NUMBER: 131:58814

TITLE: Naphthyridine derivatives of pyrrolidinylpropionic acid and analogs useful as integrin receptor antagonists

INVENTOR(S): Duggan, Mark E.; Meissner, Robert S.; Perkins, James J.

PATENT ASSIGNEE(S): Merck & Co., Inc., USA

SOURCE: PCT Int. Appl., 188 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9930709	A1	19990624	WO 1998-US26539	19981214 <--
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2315370	A1	19990624	CA 1998-2315370	19981214 <--
AU 9917257	A	19990705	AU 1999-17257	19981214 <--
AU 736026	B2	20010726		
EP 1047425	A1	20001102	EP 1998-962096	19981214 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
JP 2002508323	T	20020319	JP 2000-538692	19981214 <--
ZA 9811500	A	19990617	ZA 1998-11500	19981215 <--
US 6066648	A	20000523	US 1998-212123	19981215 <--
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of naphthyridine derivs. of pyrrolidinylpropionic acid and analogs as  $\alpha\beta 3$ ,  $\alpha\beta 5$ , and/or  $\alpha\beta 6$  integrin receptor antagonists)

IT 227938-32-1P

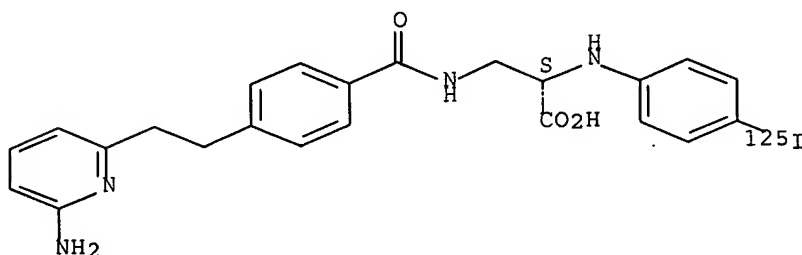
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of naphthyridine derivs. of pyrrolidinylpropionic acid and analogs as  $\alpha\beta 3$ ,  $\alpha\beta 5$ , and/or  $\alpha\beta 6$  integrin receptor antagonists)

RN 227938-32-1 HCAPLUS

CN L-Alanine, 3-[[4-[2-(6-amino-2-pyridinyl)ethyl]benzoyl]amino]-N-[4-(iodo-125I)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L167 ANSWER 14 OF 21 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:9701 HCAPLUS Full-text

DOCUMENT NUMBER: 130:81519

TITLE: Preparation of [2-(piperidin-4-yl)aminoethylcarbamoyl] substituted 1,2,3,4-tetrahydropyrimidines and oxazolidines as alpha 1a adrenergic receptor antagonists

INVENTOR(S): Patane, Michael A.; Bock, Mark G.; Newton, Randall C.

PATENT ASSIGNEE(S): Merck & Co., Inc., USA

SOURCE: PCT Int. Appl., 175 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(preparation of [2-(piperidin-4-yl)aminoethylcarbamoyl] substituted  
 1,2,3,4-tetrahydropyrimidines and oxazolidines as alpha 1a adrenergic  
 receptor antagonists)

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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)

(preparation of [2-(piperidin-4-yl)aminoethylcarbamoyl] substituted  
 1,2,3,4-tetrahydropyrimidines and oxazolidines as alpha 1a adrenergic  
 receptor antagonists)

IT 218609-83-7P 218610-00-5P

RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); RCT (Reactant); SPN (Synthetic  
 preparation); THU (Therapeutic use); BIOL (Biological study);



218610-09-4P 218610-11-8P 218610-13-0P  
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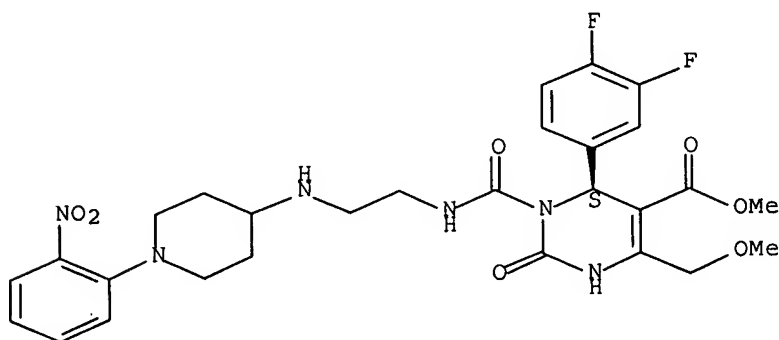
RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(preparation of [2-(piperidin-4-yl)aminoethylcarbamoyl] substituted  
 1,2,3,4-tetrahydropyrimidines and oxazolidines as alpha 1a adrenergic  
 receptor antagonists)

RN 218603-62-4 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-  
 (methoxymethyl)-1-[[[2-[[1-(2-nitrophenyl)-4-piperidiny]amino]ethyl]amino  
 ]carbonyl]-2-oxo-, methyl ester, monohydrochloride, (6S)- (9CI) (CA INDEX  
 NAME)

Absolute stereochemistry.

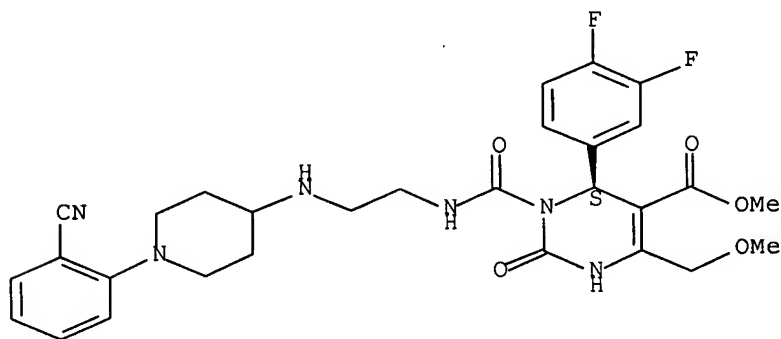


● HCl

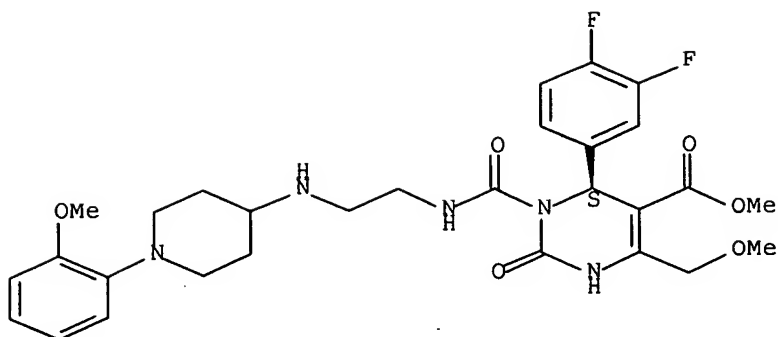
RN 218603-82-8 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-(2-cyanophenyl)-4-  
 piperidiny]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-  
 tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, monohydrochloride,  
 (6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

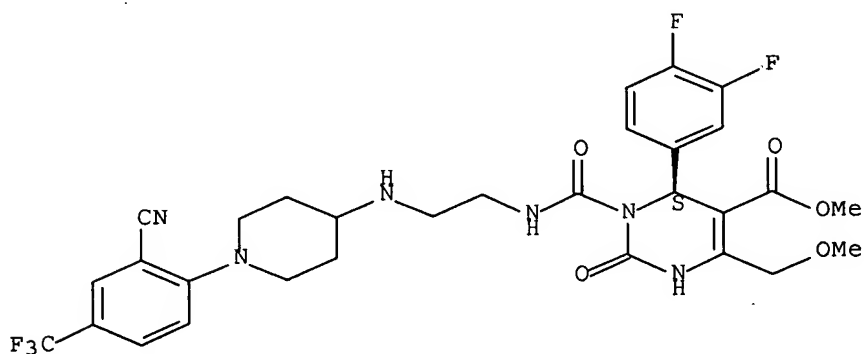


● 2 HCl

RN 218609-06-4 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-[2-cyano-4-(trifluoromethyl)phenyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, monohydrochloride, (6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

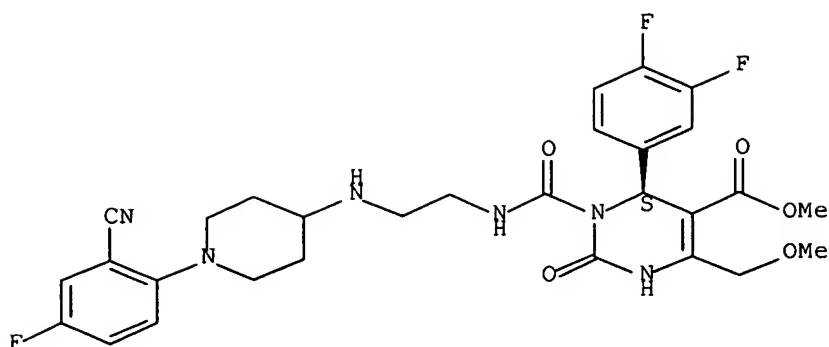


● HCl

RN 218609-07-5 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-(2-cyano-4-methylphenyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, monohydrochloride, (6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

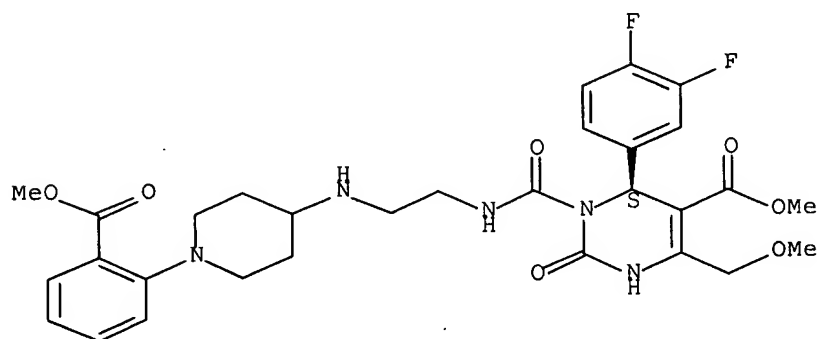


● HCl

RN 218609-10-0 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-1-[[[2-[[1-[2-(methoxycarbonyl)phenyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-4-(methoxymethyl)-2-oxo-, methyl ester, monohydrochloride, (6S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

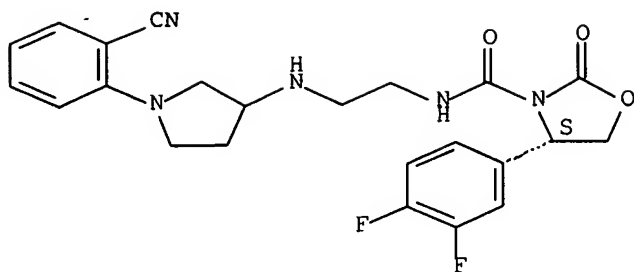


● HCl

RN 218609-12-2 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-1-[[[2-[[1-[2-(2,2,2-trifluoroethoxy)phenyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-, methyl ester, monohydrochloride, (6S)-(9CI) (CA INDEX NAME)

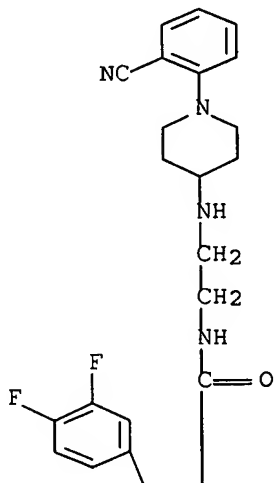
Absolute stereochemistry.



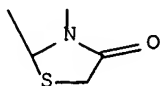
● HCl

RN 218609-15-5 HCAPLUS  
 CN 3-Thiazolidinecarboxamide, N-[2-[[1-(2-cyanophenyl)-4-piperidinyl]amino]ethyl]-2-(3,4-difluorophenyl)-4-oxo- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

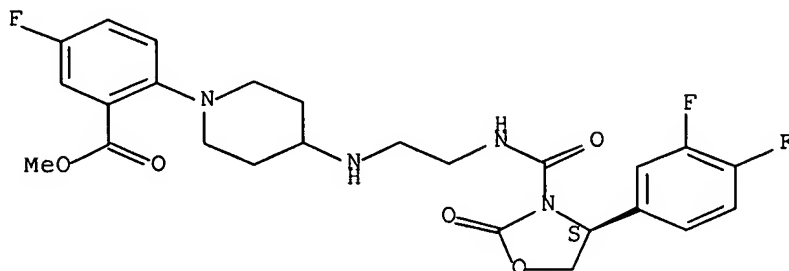


RN 218609-17-7 HCAPLUS  
 CN 3-Oxazolidinecarboxamide, N-[2-[[1-(2-cyanophenyl)-4-piperidinyl]amino]ethyl]-4-(3,4-difluorophenyl)-5-methyl-2-oxo-, (4S,5R)- (CA INDEX NAME)

Absolute stereochemistry.

oxazolidinyl]carbonyl]amino]ethyl]amino]-1-piperidinyll]-5-fluoro-, methyl ester, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

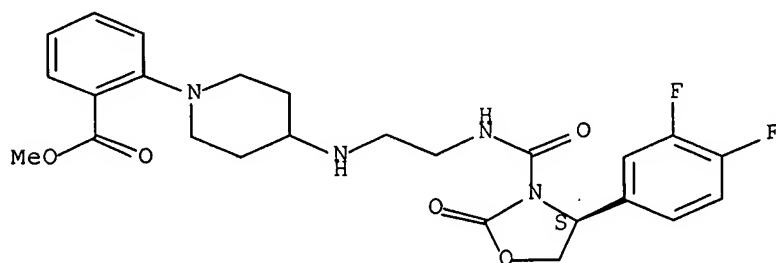


●2 HCl

RN 218609-21-3 HCAPLUS

CN Benzoic acid, 2-[4-[[2-[[[(4S)-4-(3,4-difluorophenyl)-2-oxo-3-oxazolidinyl]carbonyl]amino]ethyl]amino]-1-piperidinyll]-, methyl ester, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

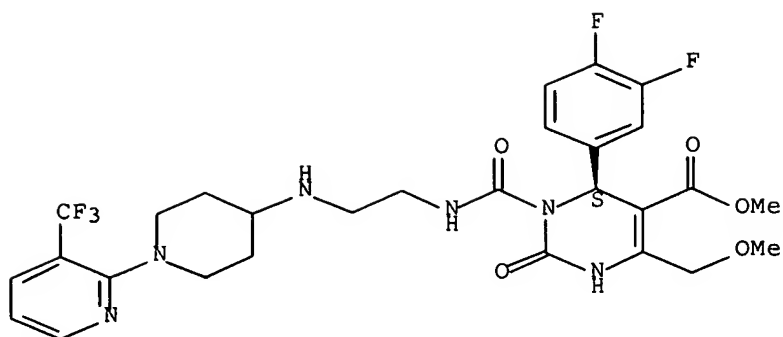


●2 HCl

RN 218609-22-4 HCAPLUS

CN 3-Oxazolidinecarboxamide, 4-(3,4-difluorophenyl)-2-oxo-N-[2-[[1-[3-(trifluoromethyl)-2-pyridinyl]-4-piperidinyll]amino]ethyl]-, (4S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 218609-26-8 HCAPLUS

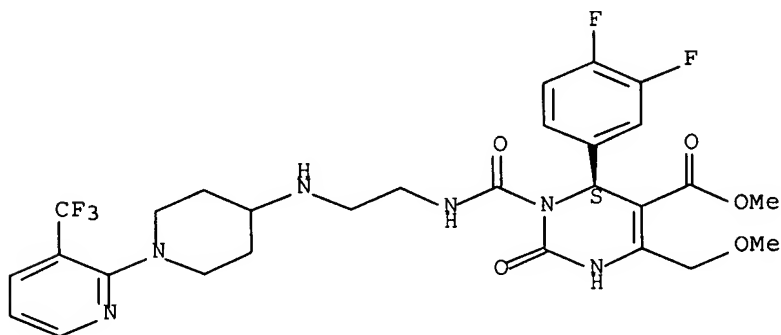
CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-1-[[[2-[[1-[3-(trifluoromethyl)-2-pyridinyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-, methyl ester, (6S)-, trifluoroacetate (2:3) (9CI) (CA INDEX NAME)

CM 1

CRN 218609-25-7

CMF C28 H31 F5 N6 O5

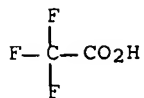
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



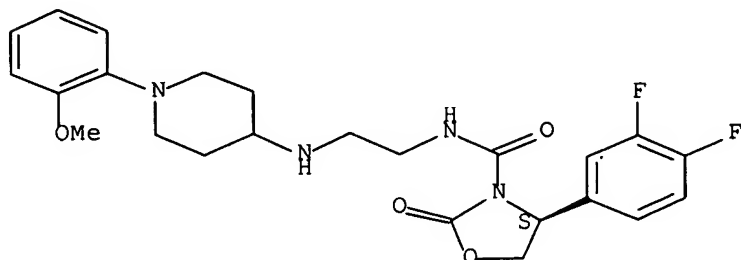
RN 218609-27-9 HCAPLUS

CN 3-Oxazolidinecarboxamide, 4-(3,4-difluorophenyl)-2-oxo-N-[2-[[1-[4-(trifluoromethyl)-2-pyrimidinyl]-4-piperidinyl]amino]ethyl]-, (4S)- (CA

RN 218609-30-4 HCAPLUS

CN 3-Oxazolidinecarboxamide, 4-(3,4-difluorophenyl)-N-[2-[[1-(2-methoxyphenyl)-4-piperidinyl]amino]ethyl]-2-oxo-, dihydrochloride, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

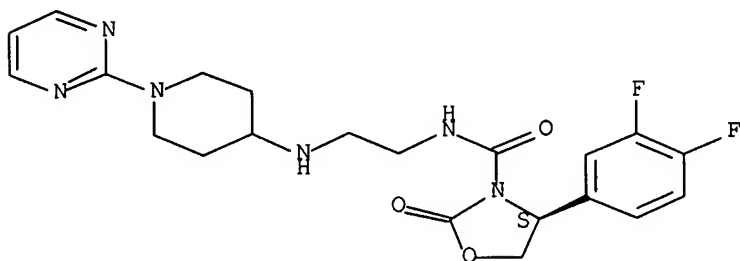


●2 HCl

RN 218609-31-5 HCAPLUS

CN 3-Oxazolidinecarboxamide, 4-(3,4-difluorophenyl)-2-oxo-N-[2-[[1-(2-pyrimidinyl)-4-piperidinyl]amino]ethyl]-, trihydrochloride, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



●3 HCl

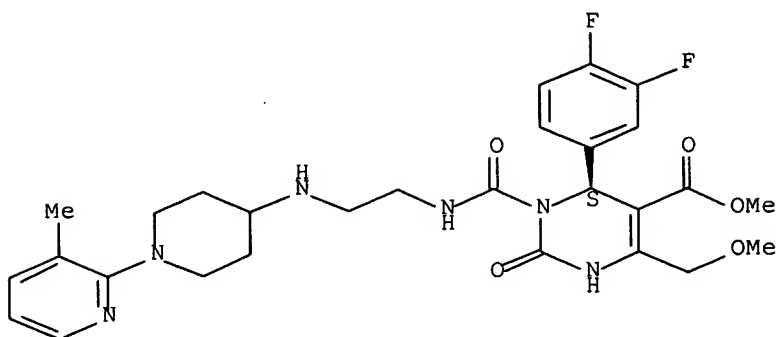
RN 218609-32-6 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-1-[[[2-[[1-[2-(trifluoromethyl)phenyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-, methyl ester, monohydrochloride, (6S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

piperidinyl]amino]ethyl]amino]carbonyl]-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

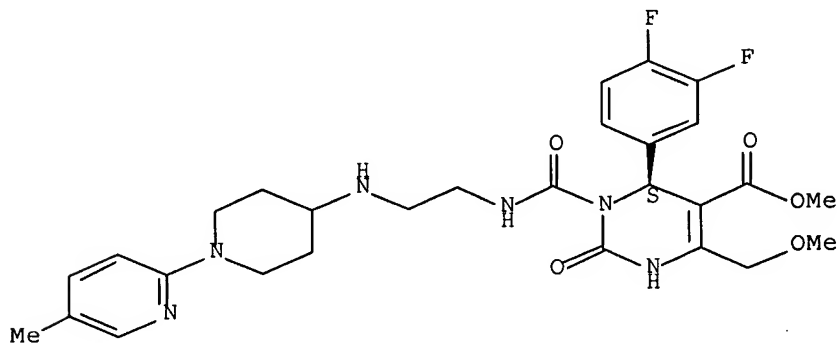
Absolute stereochemistry.



RN 218609-37-1 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-1-[[[2-[[1-(5-methyl-2-pyridinyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

Absolute stereochemistry.

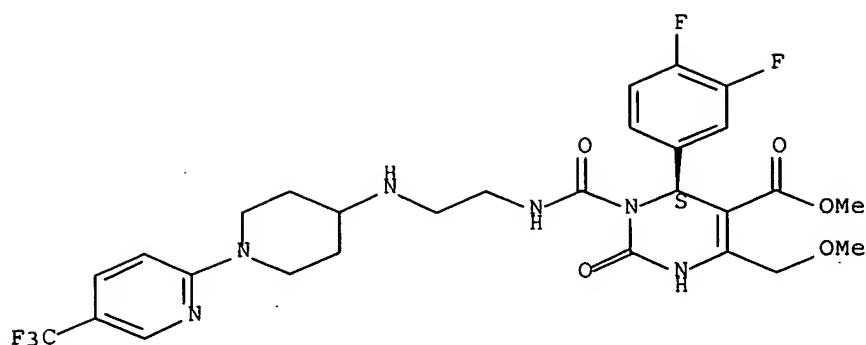


RN 218609-39-3 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-1-[[[2-[[1-(4-methoxyphenyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-2-oxo-, methyl ester, dihydrochloride, (6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





RN 218609-42-8 HCAPLUS

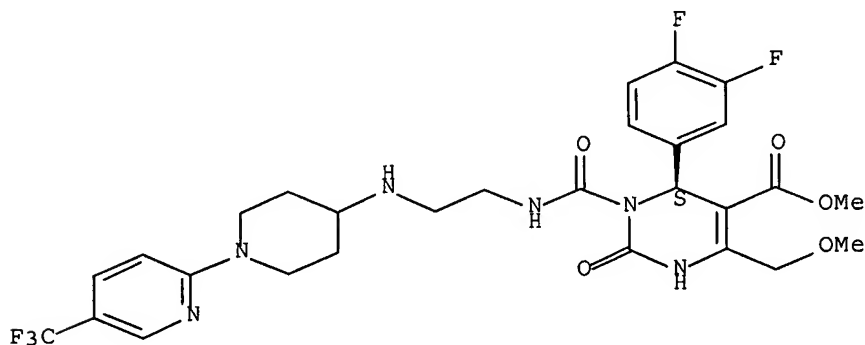
CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-1-[[[2-[[1-[5-(trifluoromethyl)-2-pyridinyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-, methyl ester, (6S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 218609-41-7

CMF C28 H31 F5 N6 O5

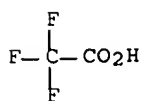
Absolute stereochemistry.



CM 2

CRN 76-05-1

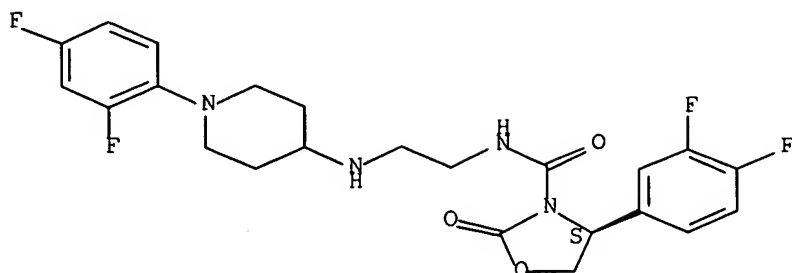
CMF C2 H F3 O2



RN 218609-43-9 HCAPLUS

CN 3-Oxazolidinecarboxamide, 4-(3,4-difluorophenyl)-2-oxo-N-[2-[[1-[5-(trifluoromethyl)-2-pyridinyl]-4-piperidinyl]amino]ethyl]-, (4S)- (CA

Absolute stereochemistry.

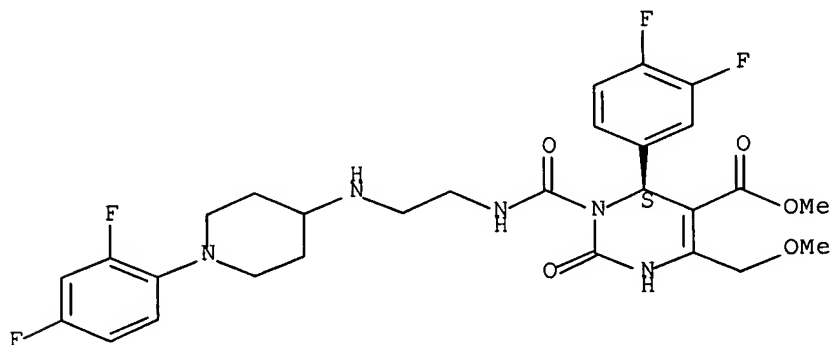


● HCl

RN 218609-46-2 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1-[[[2-[[1-(2,4-difluorophenyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, monohydrochloride, (6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

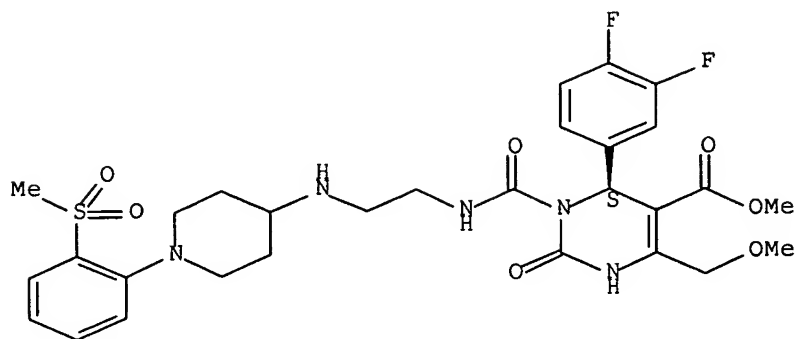
RN 218609-47-3 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-1-[[[2-[[1-[4-(trifluoromethyl)-2-pyridinyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-, methyl ester, (6S)- (CA INDEX NAME)

Absolute stereochemistry.

monohydrochloride, (6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

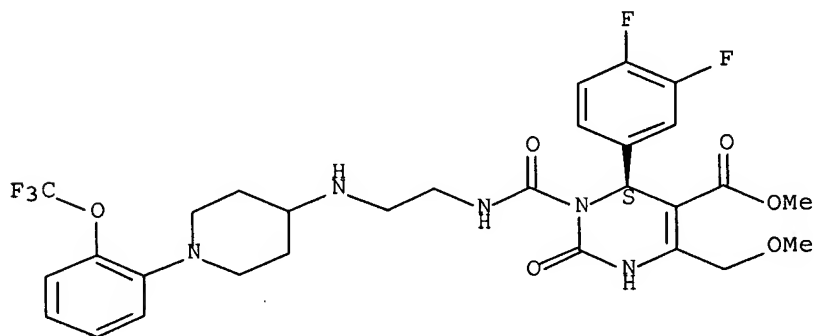


● HCl

RN 218609-52-0 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-1-[[[2-[[1-(2-(trifluoromethoxy)phenyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-, methyl ester, (6S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 218609-53-1 HCAPLUS

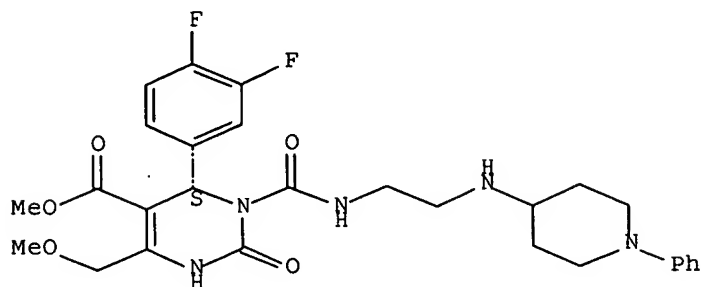
CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-(2-cyanophenyl)-3-azetidiny]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 218609-57-5 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-1-[[[2-[(1-phenyl-4-piperidinyl)amino]ethyl]amino]carbonyl]-, methyl ester, (6S)- (CA INDEX NAME)

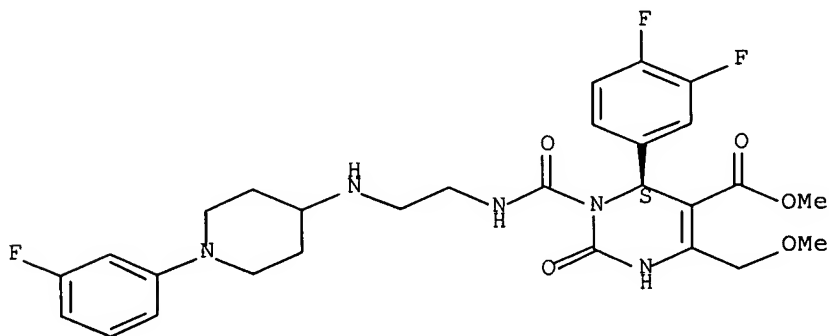
Absolute stereochemistry.



RN 218609-58-6 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1-[[[2-[[1-(3-fluorophenyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 218609-59-7 HCAPLUS

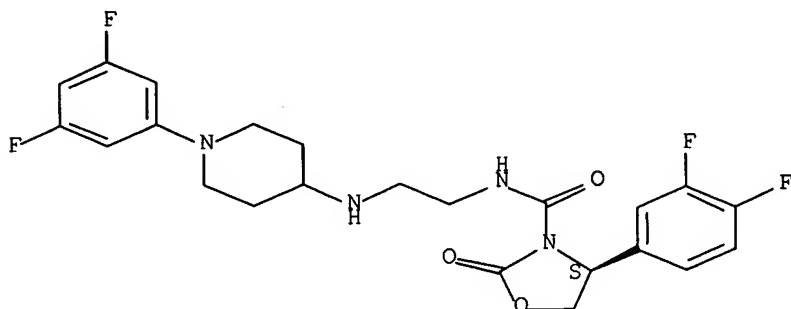
CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-1-[[[2-[[1-[4-(methoxycarbonyl)phenyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-4-(methoxymethyl)-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 218609-62-2 HCAPLUS

CN 3-Oxazolidinecarboxamide, 4-(3,4-difluorophenyl)-N-[2-[[1-(3,5-difluorophenyl)-4-piperidinyl]amino]ethyl]-2-oxo-, (4S)- (CA INDEX NAME)

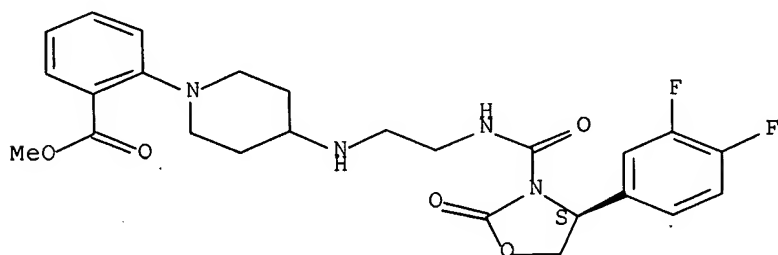
Absolute stereochemistry.



RN 218609-63-3 HCAPLUS

CN Benzoic acid, 2-[4-[[2-[[[(4S)-4-(3,4-difluorophenyl)-2-oxo-3-oxazolidinyl]carbonyl]amino]ethyl]amino]-1-piperidinyl]-, methyl ester (CA INDEX NAME)

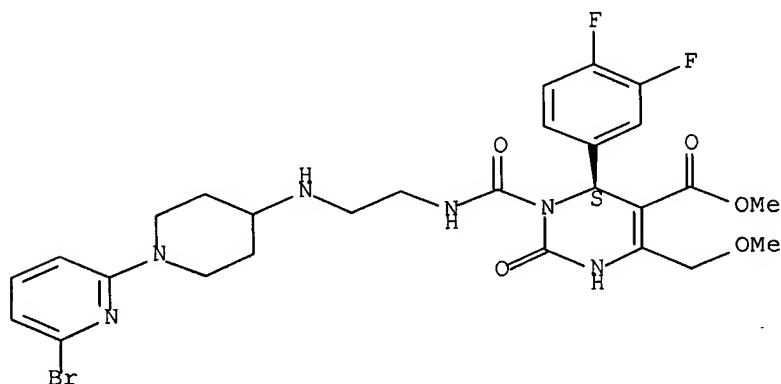
Absolute stereochemistry.

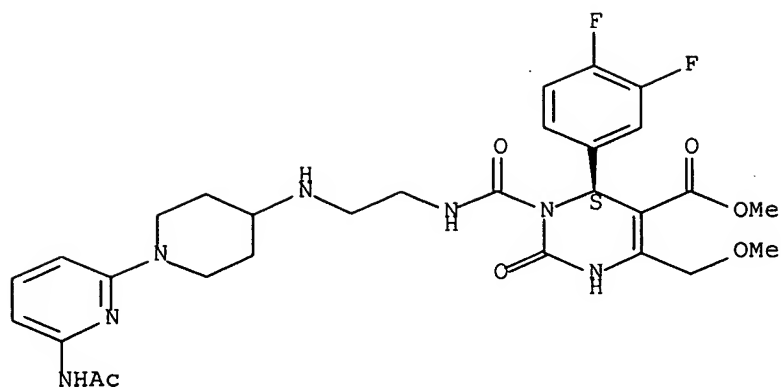


RN 218609-64-4 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-(6-bromo-2-pyridinyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

Absolute stereochemistry.

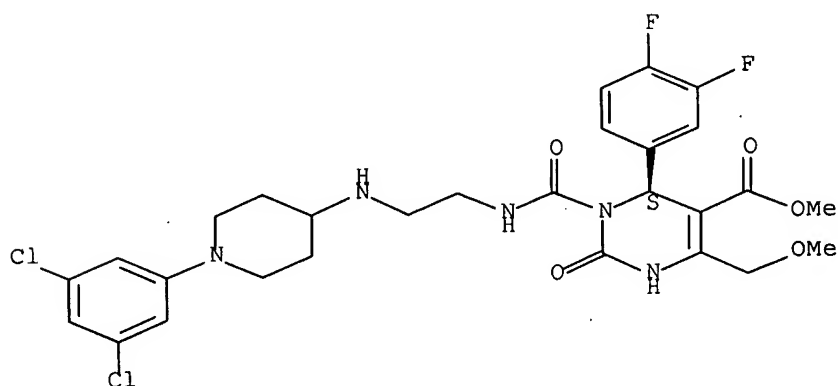




RN 218609-69-9 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-(3,5-dichlorophenyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

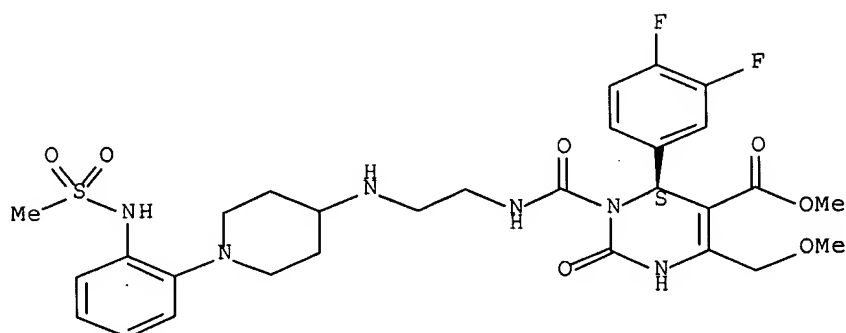
Absolute stereochemistry.

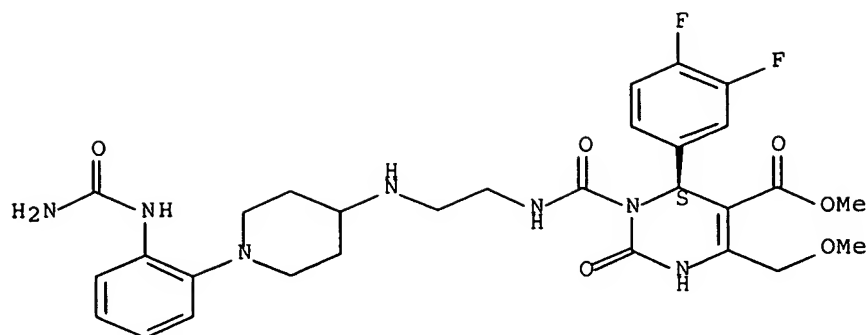


RN 218609-70-2 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-1-[[[2-[[1-[2-[(methylsulfonyl)amino]phenyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

Absolute stereochemistry.

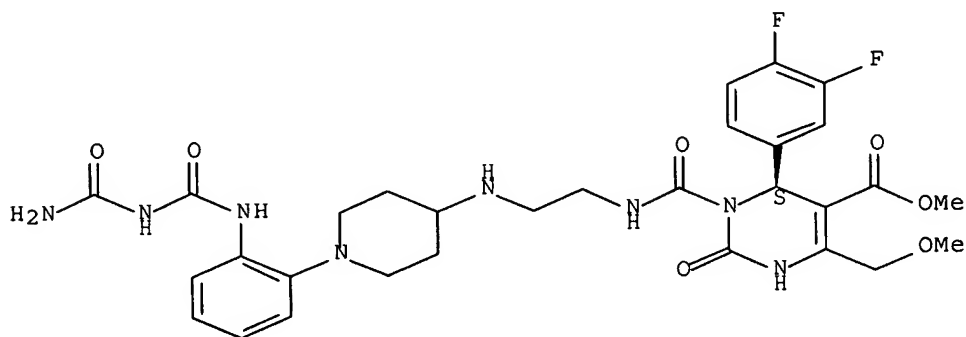




RN 218609-74-6 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-[2-[[[(aminocarbonyl)amino]carbonyl]amino]phenyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

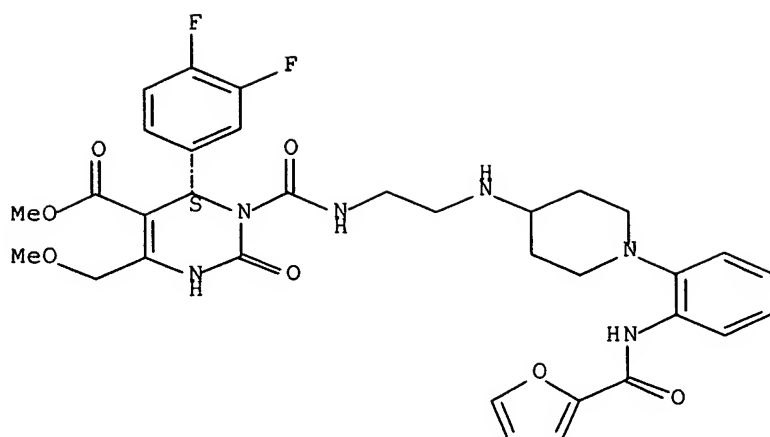
Absolute stereochemistry.



RN 218609-75-7 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-1-[[[2-[[1-(1-isoquinolinyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-4-(methoxymethyl)-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

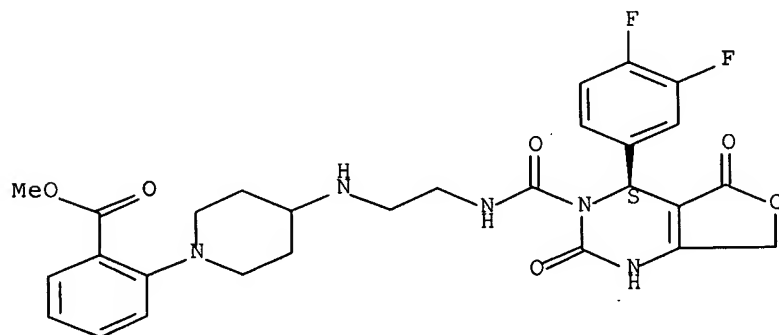
Absolute stereochemistry.



RN 218609-78-0 HCAPLUS

CN Benzoic acid, 2-[4-[[2-[[[(4S)-4-(3,4-difluorophenyl)-1,2,5,7-tetrahydro-2,5-dioxofuro[3,4-d]pyrimidin-3(4H)-yl]carbonyl]amino]ethyl]amino]-1-piperidinyl]-, methyl ester (CA INDEX NAME)

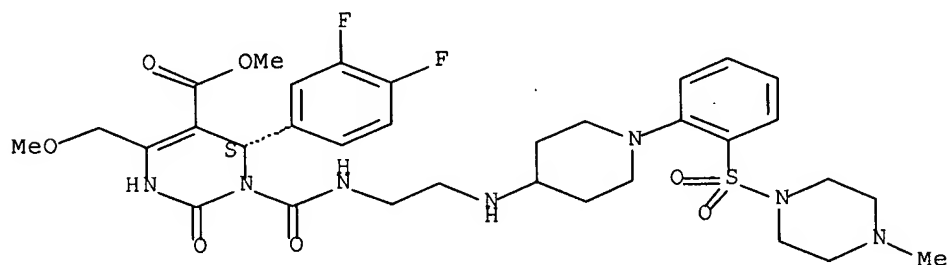
Absolute stereochemistry.



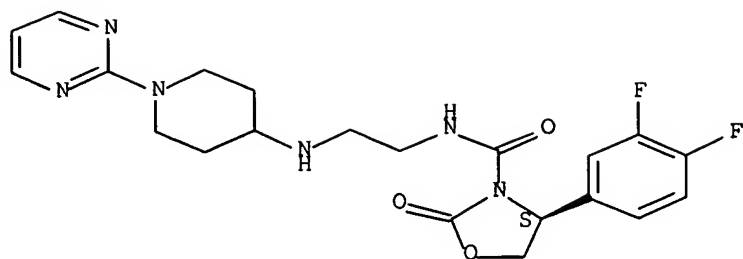
RN 218609-79-1 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-1-[[[2-[[1-[2-[(4-methyl-1-piperazinyl)sulfonyl]phenyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

Absolute stereochemistry.

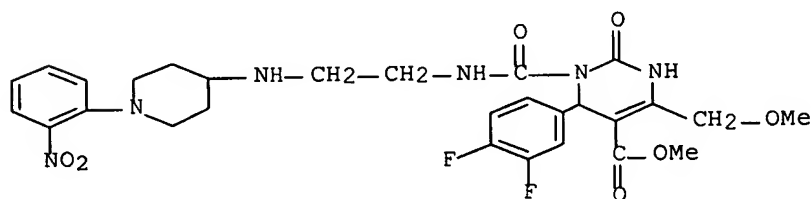






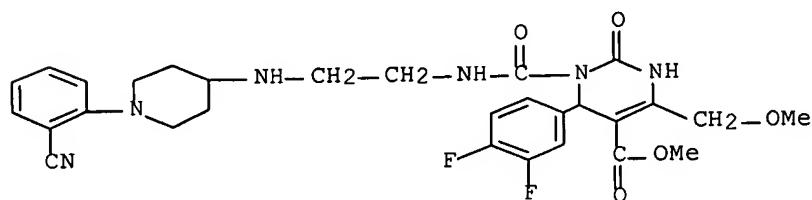
RN 218609-84-8 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-1-[[[2-[[1-(2-nitrophenyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-2-oxo-, methyl ester (CA INDEX NAME)



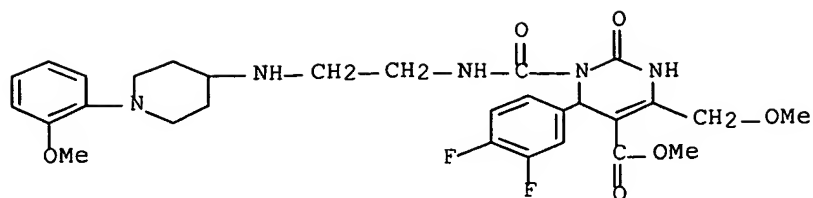
RN 218609-85-9 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-(2-cyanophenyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester (CA INDEX NAME)



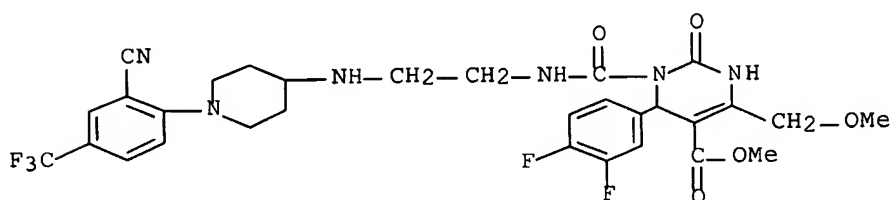
RN 218609-86-0 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-1-[[[2-[[1-(2-methylphenyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-2-oxo-, methyl ester (CA INDEX NAME)



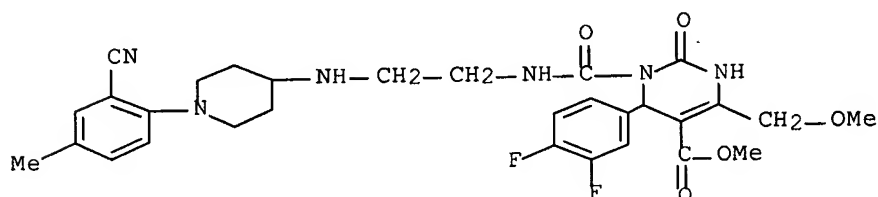
RN 218609-90-6 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-[2-cyano-4-(trifluoromethyl)phenyl]-4-piperidinyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester (CA INDEX NAME)



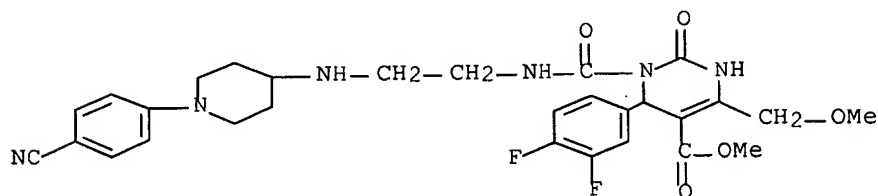
RN 218609-91-7 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-(2-cyano-4-methylphenyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester (CA INDEX NAME)

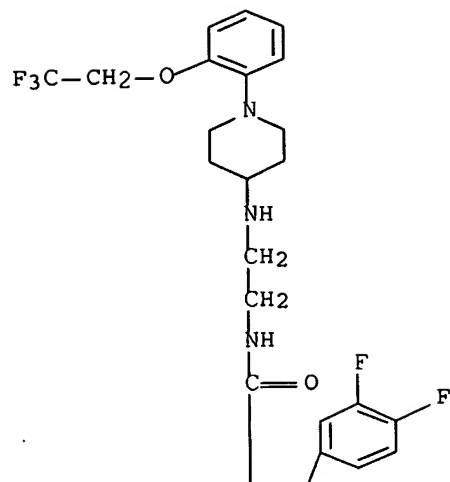


RN 218609-92-8 HCAPLUS

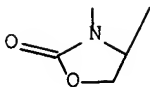
CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-(4-cyanophenyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester (CA INDEX NAME)



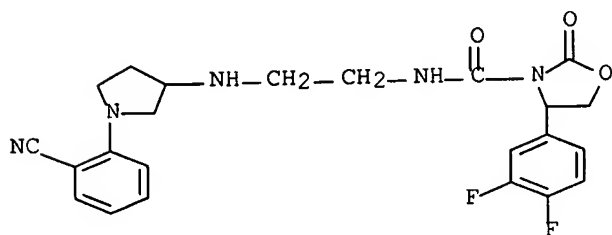
PAGE 1-A



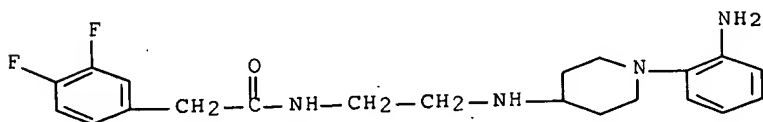
PAGE 2 - A



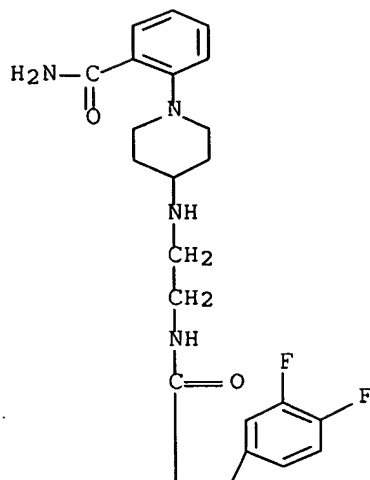
RN	218609-99-5	HCAPLUS	
CN	3-Oxazolidinecarboxamide, N-[2-[[1-(2-cyanophenyl)-3-pyrrolidinyl]amino]ethyl]-4-(3,4-difluorophenyl)-2-oxo-		(CA INDEX NAME)



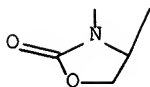
RN	218610-01-6	HCAPLUS
CN	Benzeneacetamide, N-[2-[[1-(2-aminophenyl)-4-piperidinyl]amino]ethyl]-3,4-difluoro- (CA INDEX NAME)	



PAGE 1-A

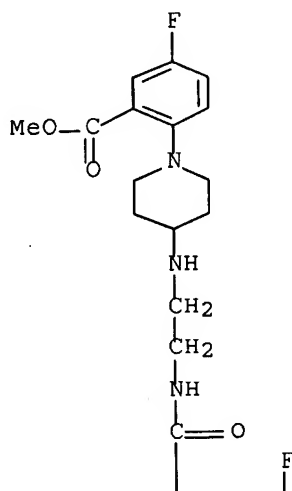


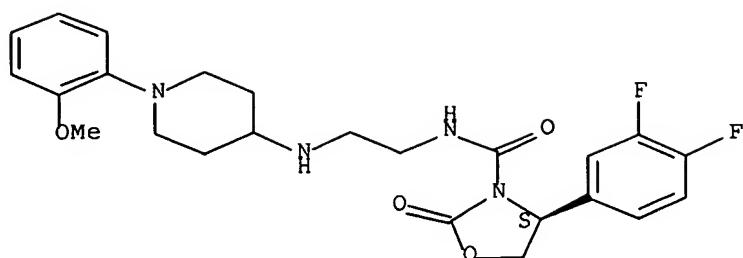
PAGE 2-A



RN 218610-07-2 HCAPLUS  
 CN Benzoic acid, 2-[4-[[2-[[[4-(3,4-difluorophenyl)-2-oxo-3-oxazolidinyl]carbonyl]amino]ethyl]amino]-1-piperidinyl]-5-fluoro-, methyl ester (CA INDEX NAME)

PAGE 1-A

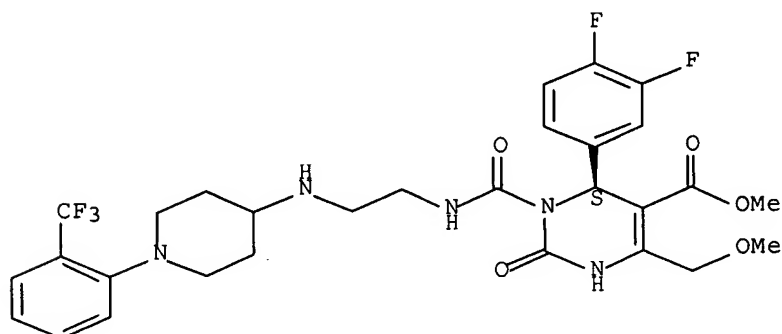




RN 218610-11-8 HCAPLUS

218610-11-8 NCAR005  
5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-1-[[[2-[[1-[2-(trifluoromethyl)phenyl]-4-piperidiny]amino]ethyl]amino]carbonyl]-, methyl ester, (6S)- (CA INDEX NAME)

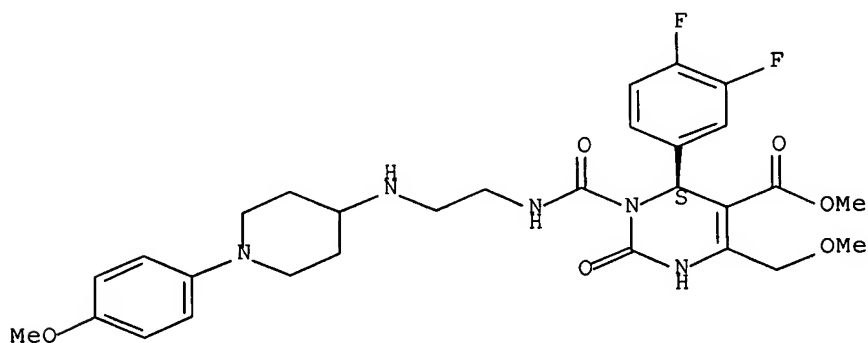
Absolute stereochemistry.



RN 218610-13-0 HCAPLUS

RN 218610-15-0 HCAFD03  
CN 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-1-[[[2-[[1-(4-methoxyphenyl)-4-piperidinyl]amino]ethyl]amino]carbonyl]-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

Absolute stereochemistry.

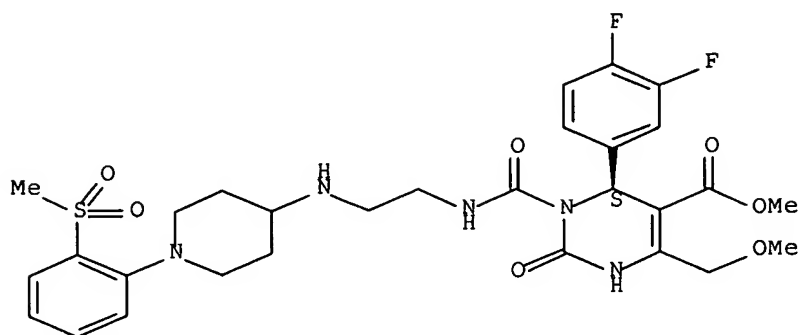


RN 218610-14-1 HCAPLUS

RN 218610-14-1 HCAFL05  
CN 3-Oxazolidinecarboxamide, 4-(3,4-difluorophenyl)-N-[2-[[1-(4-

piperidiny]amino]ethyl]amino]carbonyl]-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

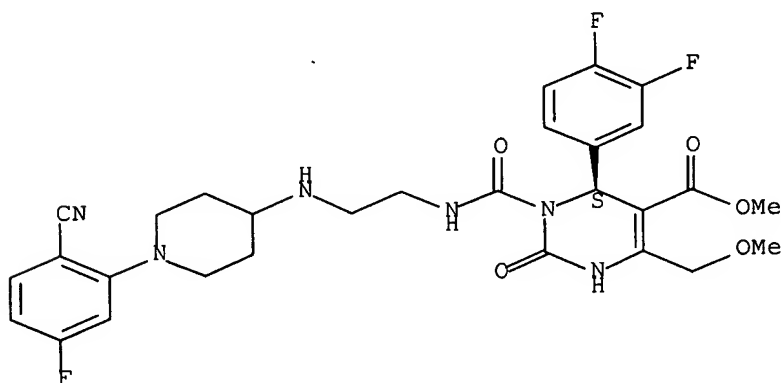
Absolute stereochemistry.



RN 218610-19-6 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-[[[2-[[1-(2-cyano-5-fluorophenyl)-4-piperidiny]amino]ethyl]amino]carbonyl]-6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4-(methoxymethyl)-2-oxo-, methyl ester, (6S)- (CA INDEX NAME)

Absolute stereochemistry.



IT 218610-66-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of [2-(piperidin-4-yl)aminoethylcarbonyl] substituted 1,2,3,4-tetrahydropyrimidines and oxazolidines as alpha 1a adrenergic receptor antagonists)

RN 218610-66-3 HCAPLUS

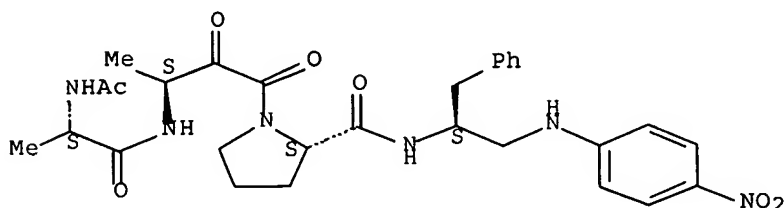
CN Benzeneacetamide, N-[2-[[1-(2-aminophenyl)-4-piperidiny]amino]ethyl]-3,4-difluoro-, trihydrochloride (9CI) (CA INDEX NAME)

peptidyl-prolyl cis-trans isomerization in the folding of RNase T1)

RN 211385-93-2 HCAPLUS

CN 2-Pyrrolidinecarboxamide, 1-[(3S)-3-[[[(2S)-2-(acetylamino)-1-oxopropyl]amino]-1,2-dioxobutyl]-N-[(1S)-1-[[[4-nitrophenyl]amino]methyl]-2-phenylethyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



IT 211385-96-5P 211385-97-6P 211385-98-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of a hapten that elicits an antibody capable of catalyzing peptidyl-prolyl cis-trans isomerization in the folding of RNase T1)

RN 211385-96-5 HCAPLUS

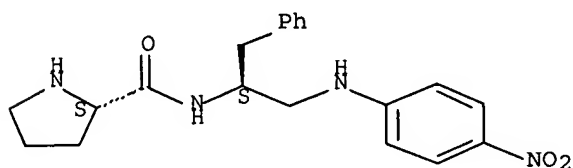
CN 2-Pyrrolidinecarboxamide, N-[(1S)-1-[[[4-nitrophenyl]amino]methyl]-2-phenylethyl]-, (2S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1.

CRN 211385-95-4

CMF C20 H24 N4 O3

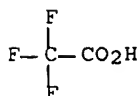
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 211385-97-6 HCAPLUS

CN Carbamic acid, [(1S,2R)-2-hydroxy-1-methyl-3-[(2S)-2-[[[(1S)-1-[[[4-

PRIORITY APPLN. INFO.:

US 1996-27764P

P 19961007 &lt;--

WO 1997-US18178

W 19971007 &lt;--

US 1999-284055

B1 19990407 &lt;--

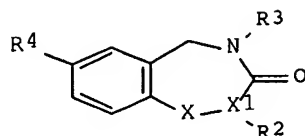
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A1 20000816 &lt;--

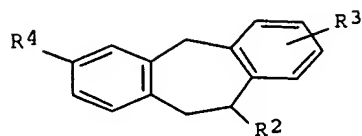
OTHER SOURCE(S):

MARPAT 128:294793

GI



I



II

AB The title compds. [I or II; X-X1 = NR1CH, N:C, CR1:C, etc.; R1 = H, C1-6 alkyl, Ar-C1-6 alkyl; R2 = (CH2)nCO2R'; R3 = H, C1-6 alkyl, Ar-C0-6 alkyl, etc.; R4 = W-(Q')p(CR'2)qU(CR'2)s; R' = H, C1-6 alkyl, C3-7 cycloalkyl, etc.; Q' = NR5, S, CR5; U = NR6C(O), C(O)NR6, CH2CO, etc.; R5, R6 = H, C1-6 alkyl, etc.; W = (un)substituted pyridyl, piperidiny, imidazolyl, etc.; n = 1-2; p = 0-1; q = 0-3; s = 0-3], integrin binding compds. which cause the release of osteocalcin from osteoblasts, and are therefore useful for treating osteoporosis, hyperparathyroidism, Paget's disease, hypercalcemia of malignancy, osteolytic lesions produced by bone metastasis, or bone loss due to immobilization or sex hormone deficiency, were prepared and formulated. Thus, treatment of Me (±)-7-carboxy-4-methyl-3-oxo-2,3,4,5-tetrahydro-1H-1,4-benzodiazepine-2-acetate with SOCl2 followed by reaction of the resulting intermediate with 2-(aminomethyl)benzimidazole·2HCl in the presence of pyridine and Et3N in CH2Cl2, and hydrolysis of the acetate with 1.0 LiOH in THF/H2O afforded the title compound I [X = NH; X1 = CH; R2 = CH2COOH; R3 = Me; R4 = {[2-benzimidazolyl)methyl]amino}carbonyl]. Prepared compds. I or II showed EC50 of < 1 μM in the ROS 17/2.8 osteocalcin assay.

IC ICM A61K031-55

ICS A61K031-555; C07D223-16; C07D243-14; C07D243-24; C07D267-14; C07D281-10

CC 28-21 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1, 63

IT	175529-27-8P	175529-28-9P	175529-29-0P	175529-34-7P	175529-37-0P
	175529-38-1P	175529-39-2P	175529-41-6P	175529-44-9P	175529-45-0P
	175529-50-7P	175529-51-8P	175529-56-3P	175529-58-5P	175529-59-6P
	175529-60-9P	175529-66-5P	175529-68-7P	175529-71-2P	175529-72-3P
	175529-75-6P	175529-76-7P	193473-11-9P	205677-90-3P	
	205677-92-5P	205678-30-4P	206113-20-4P	206113-21-5P	206113-22-6P
	206114-32-1P	206114-33-2P	206124-43-8P	206124-44-9P	206124-45-0P
	206124-46-1P	206124-47-2P	206124-48-3P	206124-64-3P	206182-50-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of benzodiazepines and dibenzo[a,d]cycloheptanes for stimulating bone formation)

IT	19614-12-1P	21901-29-1P	33259-72-2P	74764-17-3P	77605-57-3P
	77605-63-1P	77605-69-7P	81036-20-6P	90101-22-7P	92809-96-6P
	104053-68-1P	175530-10-6P	175530-11-7P	175530-12-8P	175530-13-9P
	175530-14-0P	175530-16-2P	175530-17-3P	175530-19-5P	175530-21-9P
	175530-22-0P	175530-24-2P	175530-25-3P	175530-26-4P	175530-27-5P
	175530-33-3P	175530-37-7P	175530-38-8P	175530-39-9P	175530-43-5P
	175530-46-8P	175530-47-9P	175530-48-0P	175530-49-1P	175530-55-9P



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L167 ANSWER 17 OF 21 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:248791 HCAPLUS Full-text

DOCUMENT NUMBER: 126:327291

TITLE: Design of kallidin-releasing tissue kallikrein inhibitors based on the specificities of the enzyme's binding subsites

AUTHOR(S): Portaro, Fernanda C. V.; Cezari, Maria H. S.; Juliano, Maria A.; Juliano, Luiz; Walmsley, Adrian R.; Prado, Eline S.

CORPORATE SOURCE: Department Biophysics, Universidade Federal Sao Paulo-Escola Paulista Medicina, Sao Paulo, 04044-020, Brazil

SOURCE: Biochemical Journal (1997), 323(1), 161-171

CODEN: BIJOAK; ISSN: 0264-6021

PUBLISHER: Portland Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Tissue kallikrein inhibitors were derived by selectively replacing residues in Na-substituted arginine- or phenylalanine-pNA ( where pNA is p-nitroanilide), and in peptide substrates for these enzymes. Phenylacetyl-Arg-pNA was an efficient inhibitor of human tissue kallikrein ( $K_i$  0.4  $\mu$ M) and was neither a substrate nor an inhibitor of plasma kallikrein. The peptide inhibitors having phenylalanine as the P1 residue behaved as specific inhibitors for kallidin-releasing tissue kallikreins, whereas plasma kallikrein showed high affinity for inhibitors containing (p-nitro)phenylalanine at the same position. The  $K_i$  value of the most potent inhibitor developed, Abz-Phe-Arg-Arg-Pro-Arg- EDDnp [where Abz is o-aminobenzoyl and EDDnp is N-(2,4-dinitrophenyl)- ethylenediamine], was 0.08  $\mu$ M for human tissue kallikrein. Progress curve analyses of the inhibition of human tissue kallikrein by benzoyl-Arg-pNA and phenylacetyl-Phe-Ser-Arg-EDDnp indicated a single-step mechanism for reversible formation of the enzyme-inhibitor complex.

CC 7-3 (Enzymes)

IT 965-03-7, Benzoyl-L-argininamide 971-21-1, Benzoyl-L-arginine, ethyl ester 6208-93-1, Benzoyl-L-arginine p-nitroanilide 29618-30-2  
72150-35-7 110084-85-0 133839-14-2 133839-16-4 133839-17-5  
162851-95-8 162851-96-9 179166-90-6 179166-91-7 179166-92-8  
179166-98-4 189621-36-1 189621-37-2 189621-38-3 189621-39-4  
189621-40-7 189621-41-8 189621-42-9 189621-43-0 189621-44-1  
189621-45-2 189621-46-3 189621-47-4 189621-48-5 189621-49-6  
189621-50-9 189621-51-0 189621-52-1 189621-53-2 189621-54-3  
189621-55-4 189633-09-8

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(design of kallidin-releasing tissue kallikrein inhibitors based on the specificities of the enzyme's binding subsites)

IT 133839-17-5

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

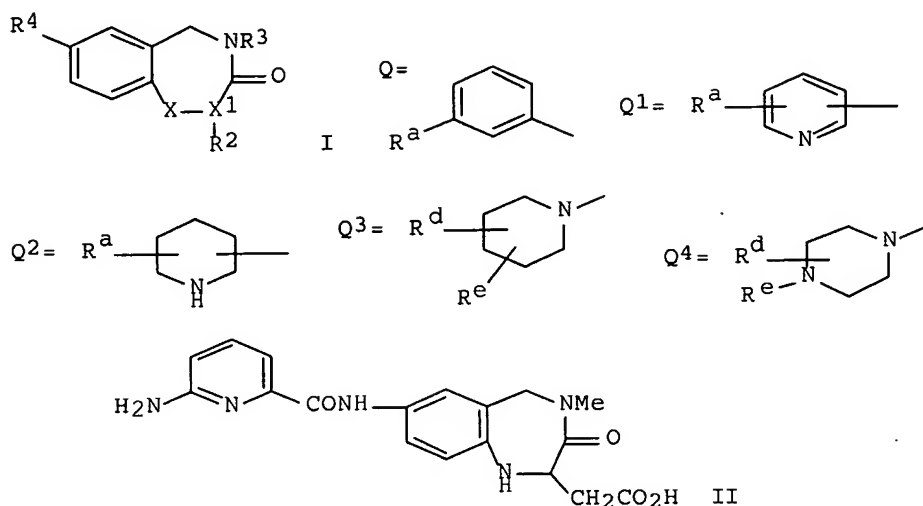
(design of kallidin-releasing tissue kallikrein inhibitors based on the specificities of the enzyme's binding subsites)

RN 133839-17-5 HCAPLUS

CN L-Prolinamide, N-(2-aminobenzoyl)-L-phenylalanyl-L-arginyl-L-arginyl-N-[2-

JP 10504807 T 19980512 JP 1995-503418 19950629 <--  
 US 6458784 B1 20021001 US 2000-679982 20001005 <--  
 PRIORITY APPLN. INFO.: US 1994-267695 A 19940629 <--  
 WO 1995-US8146 W 19950629 <--  
 US 1996-765753 B1 19961220 <--  
 US 1998-482647 B1 19981110 <--

OTHER SOURCE(S): MARPAT 124:289585  
 GI



AB The title compds. [I; X-X1 = NR1CH, NC(O)R3-CH, N:C, CR1:C, CHR1-CH, O-CH or S-CH; wherein R1 = H, C1-6 alkyl, benzyl; R2 = (CH2)nCO2H; R3 = H, C1-6 alkyl, Ar-CO-6 alkyl, Het-CO-6 alkyl, C3-6 cycloalkyl-CO-6 alkyl; wherein Ar and Het are not defined; R4 = W-U, Y-(CHR5)m-U or Z-C(O); R5, R6 = H, C1-6 alkyl, Ar-CO-6 alkyl, Het-CO-6 alkyl, C3-6 cycloalkyl-CO-6 alkyl; m, n = 1, 2; U = NR1C(O), C(O)NR1, CH:CH, C.tplbond.C, CH2-CH2, O-CH2, CH2-O, CH2O2CNR1; W = Q, Q1, Q2; wherein Ra = H, OH, NO2, N(R6)2, CON(R6)2, CH2N(R6)2, R6HN-C(:NH); Y = NH2, NHR6, N(R6)2, C(O)N(R6)2, OH, :N-OR6, 3-Q2, 2- or 3-Q1; Z = Q3, Q4; Rd = H, N(R1)2, C1-4 alkyl, CON(R1)2, OH, OR1, Ar-CO-4alkyl; Re = H, C1-4 alkyl, 2- or 3-pyridinyl, 1-, 2- or 3-piperidinyl, or 2- or 4-pyrimidinyl] and pharmaceutically acceptable salts thereof, which are useful for treating osteoporosis, atherosclerosis, cancer, or restenosis in a mammal, are prepared. Thus, Me 7-carboxy-4-methyl-3-oxo-2,3,4,5-tetrahydro-1H-1,4-benzodiazepine-2-acetate was condensed with 2,6-diaminopyridine using 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride and HOBT.H2O in DMF to give, after saponification with LiOH in aqueous THF, the title compound (II), which showed Ki (dissociation constant) of 0.15  $\mu$ M in solid phase [3H]-SK&F-107260 binding to human placenta or human platelet  $\alpha$ v $\beta$ 3.

IC ICM A61K031-55

ICS C07D243-14

CC 28-21 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1

IT 175532-77-1P 175532-78-2P 175532-79-3P 175532-80-6P 175532-81-7P  
 175532-82-8P 175532-83-9P 175532-84-0P 175532-85-1P 175532-86-2P  
 175532-87-3P 175532-88-4P 175532-89-5P 175532-90-8P 175532-91-9P  
 175532-92-0P 175532-93-1P 175532-94-2P 175532-95-3P  
 175532-96-4P 175532-97-5P 175532-98-6P 175672-22-7P

DOCUMENT NUMBER: 121:272191  
 TITLE: Oxoquinolinecarboxylic acid derivatives,  
 oxonaphthyridinecarboxylic acid derivatives, their  
 preparation, and their use as cell adhesion inhibitors  
 INVENTOR(S): Miyake, Akio; Nakamura, Masahira; Fukushi, Hideto  
 PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan  
 SOURCE: Eur. Pat. Appl., 49 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 614664	A1	19940914	EP 1994-103366	19940305 <--
EP 614664	B1	19980916		
EP 614664	B2	20030108		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
AU 9456437	A	19940915	AU 1994-56437	19940228 <--
AU 669416	B2	19960606		
AT 171068	T	19981015	AT 1994-103366	19940305 <--
NO 9400789	A	19940912	NO 1994-789	19940307 <--
JP 06316522	A	19941115	JP 1994-35879	19940307 <--
CA 2117224	A1	19940910	CA 1994-2117224	19940308 <--
FI 9401082	A	19940910	FI 1994-1082	19940308 <--
US 5519024	A	19960521	US 1994-207091	19940308 <--
CN 1099029	A	19950222	CN 1994-102273	19940309 <--
HU 70043	A2	19950928	HU 1994-703	19940309 <--
US 5703081	A	19971230	US 1996-608697	19960229 <--
US 5889009	A	19990330	US 1997-931453	19970917 <--
US 5889009	C1	20020507		

PRIORITY APPLN. INFO.:  
 JP 1993-47917 A 19930309 <--  
 US 1994-207091 A3 19940308 <--  
 US 1996-608697 A3 19960229 <--

OTHER SOURCE(S): CASREACT 121:272191; MARPAT 121:272191

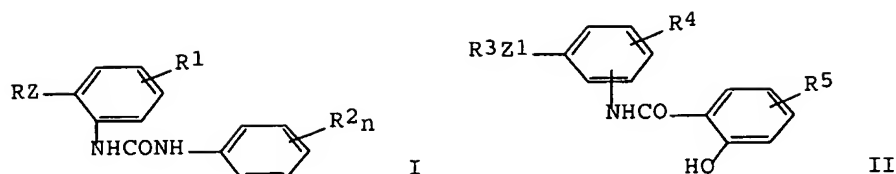
AB Compns. are disclosed which include a 1,7-disubstituted-4-oxo-3-quinolinecarboxylic acid or 1,7-disubstituted-4-oxo-3-naphthyridinecarboxylic acid derivative (Markush included). The compds. of the invention are useful as prophylactic and/or therapeutic agents for peripheral arterial obstruction, acute myocardial infarction, antitumor agents, and as prophylactic and/or therapeutic agents for osteoporosis. Preparation of compds. of the invention is described. 6,8-Difluoro-7-(4-methylpiperazin-1-yl)-1-(thiazol-2-yl)methyl-1,4-dihydro-4-oxoquinoline-3-carboxylic acid hydrochloride (I) was prepared from 1-(thiazol-2-yl)methyl-6,7,8-trifluoro-1,4-dihydro-4-oxoquinoline-3-carboxylic acid and 4-methylpiperazine. Tablet and injection formulations of I are included, as is inhibitory activity against binding of GPIIb/IIIa and fibrinogen for I and other compns. of the invention.

IC ICM A61K031-47  
 ICS C07D417-06; C07D417-14; C07D401-12; C07D401-14; C07D215-56;  
 C07D487-04; C07D519-00; C07D401-06; C07D401-04; C07D513-04

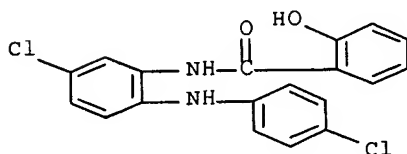
CC 1-12 (Pharmacology)  
 Section cross-reference(s): 27, 28, 63

IT Pharmaceutical dosage forms  
 (injections, oxoquinolinecarboxylic acid derivs.,  
 oxonaphthyridinecarboxylic acid derivs., their preparation, and their use  
 as  
 cell adhesion inhibitors)

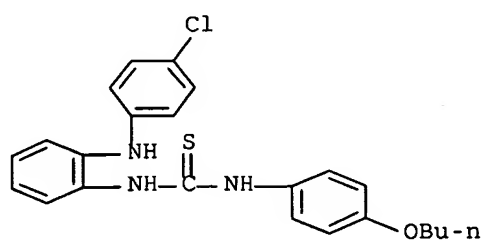
IT Pharmaceutical dosage forms  
 (tablets, oxoquinolinecarboxylic acid derivs.,



- AB Carbanilides I [R = (un)substituted Ph, naphthyl; R1 = halo, NO<sub>2</sub>, CF<sub>3</sub>; R2n = 2,2-Cl<sub>2</sub>, 2,4-Cl<sub>2</sub>; Z = O, S] and salicylanilides II (R3 = naphthyl, 4-ClC<sub>6</sub>H<sub>4</sub>; R4, R5 = H, Cl; Z1 = O, S, NH) were prepared from aryloxyanilines by condensation with dichloropheny isocyanates and salicylic acids. I (R = 1-naphthyl, R1 = 4-CF<sub>3</sub>, R2n = 2,4-Cl<sub>2</sub>, Z = O) has a min. inhibitory concentration of 0.16 µg/mL against *Staphylococcus aureus*.
- CC 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds).  
Section cross-reference(s): 1
- IT 79567-30-9P 84978-94-9P 84978-95-0P 84978-96-1P 84978-97-2P  
84978-98-3P 84978-99-4P 84979-00-0P 84979-01-1P 84979-02-2P  
84979-03-3P 84979-04-4P 84979-05-5P 84979-06-6P 84979-07-7P  
84979-08-8P 84979-09-9P 84979-10-2P 84979-11-3P 84979-12-4P  
84979-13-5P 84979-14-6P 84979-15-7P 84979-16-8P 84979-17-9P  
84979-18-0P 84979-19-1P 84979-20-4P 84979-21-5P 84979-22-6P  
84979-23-7P 84979-24-8P 84979-25-9P 84979-26-0P  
84979-27-1P 84979-28-2P 84979-29-3P  
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and bactericidal activity of)
- IT 84979-25-9P  
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and bactericidal activity of)
- RN 84979-25-9 HCAPLUS
- CN Benzamide, N-[5-chloro-2-[(4-chlorophenyl)amino]phenyl]-2-hydroxy- (CA INDEX NAME)



L167 ANSWER 21 OF 21 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1970:41258 HCAPLUS Full-text  
 DOCUMENT NUMBER: 72:41258  
 ORIGINAL REFERENCE NO.: 72:7559a,7562a  
 TITLE: Tuberculostatic 1,3-diarylthioureas. I  
 AUTHOR(S): Winkelmann, Erhardt; Wagner, Wolf H.; Hilmer, Hans  
 CORPORATE SOURCE: Farbwerke Hoechst A.-G., Frankfurt/M.-Hoechst, Fed. Rep. Ger.  
 SOURCE: Arzneimittel-Forschung (1969), 19(4), 543-58



=> s 1162 not 196,1163,1164,1165,1167  
 L168 9 L162 NOT (L96 OR L163 OR L164 OR L165 OR L167)

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L168 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2002:157734 HCAPLUS Full-text  
 DOCUMENT NUMBER: 136:200019  
 TITLE: Preparation of N-(acylaminophenyl)thioureas as  
 vanilloid receptor antagonists  
 INVENTOR(S): Suh, Young Ger; Oh, Uh Taek; Kim, Hee Doo; Lee, Jee  
 Woo; Park, Hyeung Geun; Park, Young Ho; Yi, Jung Bum  
 PATENT ASSIGNEE(S): Pacific Corporation, S. Korea  
 SOURCE: PCT Int. Appl., 55 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002016319	A1	20020228	WO 2001-KR1408	20010820 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 200180230	A	20020304	AU 2001-80230	20010820 <--
KR 2002030009	A	20020422	KR 2001-50093	20010820 <--
EP 1311478	A1	20030521	EP 2001-958603	20010820 <--
EP 1311478	B1	20060607		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004506714	T	20040304	JP 2002-521195	20010820 <--
AT 328868	T	20060615	AT 2001-958603	20010820 <--
ES 2266227	T3	20070301	ES 2001-1958603	20010820 <--
US 2003212140	A1	20031113	US 2003-362079	20030220 <--
US 7067553	B2	20060627		
KR 2004044431	A	20040528	KR 2004-32384	20040507 <--
KR 2004048393	A	20040609	KR 2004-36719	20040524 <--
KR 2005090356	A	20050913	KR 2005-78835	20050826 <--
KR 2005090357	A	20050913	KR 2005-78842	20050826 <--
PRIORITY APPLN. INFO.:			KR 2000-48385	A 20000821 <--
			KR 2000-48388	A 20000821 <--
			KR 2000-85126	A 20001229 <--
			KR 2001-50092	A3 20010820
			KR 2001-50093	A3 20010820
			WO 2001-KR1408	W 20010820
			KR 2004-32384	A3 20040507
OTHER SOURCE(S):			MARPAT 136:200019	
GI				

BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

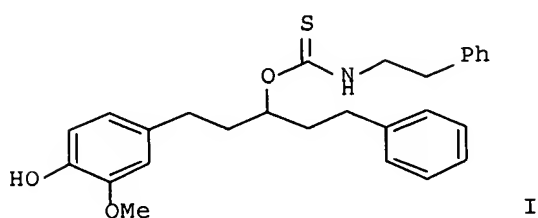
AU 2001078821	A5	20020304	AU 2001-78821	20010820 <--
KR 2002030010	A	20020422	KR 2001-50094	20010820 <--
EP 1311477	A1	20030521	EP 2001-957037	20010820 <--

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

US 2003203944	A1	20031030	US 2003-343703	20030203 <--
US 2006264480	A1	20061123	US 2006-373828	20060313 <--

PRIORITY APPLN. INFO.: KR 2000-48387 A 20000821 <--  
WO 2001-KR1409 W 20010820  
US 2003-343703 B1 20030203

OTHER SOURCE(S): MARPAT 136:216540  
GI



- AB The title compds. ArACH<sub>2</sub>CHR<sub>2</sub>ZC(:Y)NHR<sub>1</sub> [R<sub>1</sub> = (CH<sub>2</sub>)<sub>m</sub>Ar<sub>1</sub> (Ar<sub>1</sub> = (un)substituted Ph, pyridyl, thiophenyl, naphthyl; m = 1-4), (CH<sub>2</sub>)<sub>n</sub>CHPh<sub>2</sub>, (CH<sub>2</sub>)<sub>2</sub>CHPhCH<sub>2</sub>Ph (n = 1-2); Y = S, O; Z = O, CH<sub>2</sub>, NR<sub>3</sub>, CHR<sub>3</sub> (R<sub>3</sub> = H, alkyl, CH<sub>2</sub>Ph, (CH<sub>2</sub>)<sub>2</sub>Ph); R<sub>2</sub> = H, alkyl, cycloalkyl, etc.; A = O, CH<sub>2</sub>; Ar = (un)substituted Ph, pyridyl, indolyl, imidazolyl], useful as antagonists against vanilloid receptor, were prepared. E.g., a multi-step synthesis of I which showed antagonistic potency equal to capsaizipine in patchclamp test for vanilloid receptor activity, was given. As diseases associated with the activity of vanilloid receptor, pain, acute pain, chronic pain, neuropathic pain, post-operative pain, migraine, arthralgia, neuropathies, nerve injury, diabetic neuropathy, neurodegeneration, neurotic skin disorder, stroke, urinary bladder hypersensitiveness, irritable bowel syndrome, a respiratory disorder such as asthma or chronic obstructive pulmonary disease, irritation of skin, eye or mucous membrane, fevescence, stomach-duodenal ulcer, inflammatory bowel disease and inflammatory diseases can be enumerated. The present invention provides a pharmaceutical composition for prevention or treatment of these diseases.
- IC ICM C07C333-02  
ICS A61K031-075; A61K031-135
- CC 25-21 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
Section cross-reference(s): 1
- ST thiocarbamic acid prepn vanilloid receptor antagonist analgesic  
antiinflammatory
- IT Disease, animal  
Pain  
(arthralgia, treatment of; preparation of novel thiocarbamic acid derivs.  
as  
vanilloid receptor antagonists)
- IT Nerve, disease  
(neuropathy, treatment of; preparation of novel thiocarbamic acid  
derivs. as vanilloid receptor antagonists)

Anandamide-Facilitated Transport and Bind to CB1 Cannabinoid Receptors

AUTHOR(S): Melck, Dominique; Bisogno, Tiziana; De Petrocellis, Luciano; Chuang, Huai-hu; Julius, David; Bifulco, Maurizio; Di Marzo, Vincenzo

CORPORATE SOURCE: Istituto per la Chimica di Molecole di Interesse Biologico, Consiglio Naz. Ric., Arco Felice, Napoli, 80072, Italy

SOURCE: Biochemical and Biophysical Research Communications (1999), 262(1), 275-284  
CODEN: BBRC9; ISSN: 0006-291X

PUBLISHER: Academic Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We investigated the effect of changing the length and degree of unsatn. of the fatty acyl chain of N-(3-methoxy-4-hydroxy)-benzyl-cis-9-octadecenoamide (olvanil), a ligand of vanilloid receptors, on its capability to: (i) inhibit anandamide-facilitated transport into cells and enzymic hydrolysis, (ii) bind to CB1 and CB2 cannabinoid receptors, and (iii) activate the VR1 vanilloid receptor. Potent inhibition of [<sup>14</sup>C]anandamide accumulation into cells was achieved with C20:4 n-6, C18:3 n-6 and n-3, and C18:2 n-6 N-acyl-vanillyl-amides (N-AVAMs). The saturated analogs and Δ<sup>9</sup>-trans-olvanil were inactive. Activity in CB1 binding assays increased when increasing the number of cis-double bonds in a n-6 fatty acyl chain and, in saturated N-AVAMs, was not greatly sensitive to decreasing the chain length. The C20:4 n-6 analog (arvanil) was a potent inhibitor of anandamide accumulation (IC<sub>50</sub> = 3.6 μM) and was 4-fold more potent than anandamide on CB1 receptors (K<sub>i</sub> = 0.25-0.52 μM), whereas the C18:3 n-3 N-AVAM was more selective than arvanil for the uptake (IC<sub>50</sub> = 8.0 μM) vs. CB1 receptors (K<sub>i</sub> = 3.4 μM). None of the compds. efficiently inhibited [<sup>14</sup>C]anandamide hydrolysis or bound to CB2 receptors. All N-AVAMs activated the cation currents coupled to VR1 receptors overexpressed in *Xenopus* oocytes. In a simple, intact cell model of both vanilloid- and anandamide-like activity, i.e., the inhibition of human breast cancer cell (HBCC) proliferation, arvanil was shown to behave as a "hybrid" activator of cannabinoid and vanilloid receptors. (c) 1999 Academic Press.

CC 1-3 (Pharmacology)

IT Analgesics  
(effects of unsatd. long-chain N-acyl-vanillyl-amides on anandamide action and vanilloid/CB1 cannabinoid receptors in relation to analgesics)

IT Capsaicin receptors  
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(unsatd. long-chain N-acyl-vanillyl-amides as vanilloid receptor ligands that inhibit anandamide-facilitated transport and bind to CB1 cannabinoid receptors)

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L168 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:130120 HCAPLUS Full-text

DOCUMENT NUMBER: 130:347278

TITLE: Vanilloid receptor agonists potentiate the in vivo local anesthetic activity of percutaneously injected site 1 sodium channel blockers

AUTHOR(S): Kohane, Daniel S.; Kuang, Yu; Lu, Nu T.; Langer, Robert; Strichartz, Gary R.; Berde, Charles B.

CORPORATE SOURCE: Department of Anesthesia, Children's Hospital, Boston, MA, USA



W: CA, JP, US

RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,  
PT, SE

CA 2295089 A1 19990107 CA 1998-2295089 19980618 &lt;--

EP 1003491 A1 20000531 EP 1998-936402 19980618 &lt;--

R: BE, CH, DE, ES, FR, GR, IT, LI, NL

JP 2002511866 T 20020416 JP 1999-505296 19980618 &lt;--

PRIORITY APPLN. INFO.: GB 1997-13484 A 19970627 &lt;--

WO 1998-EP4005 W 19980618 &lt;--

AB The use of antagonist or partial agonists of the vanilloid receptor complexes such as capsazepine or olvanil for the treatment of neurodegenerative diseases is described. The neuroprotectant activity of the vanilloid compds., capsazepine and olvanil to protect the neuronal HT-4 cell line from glutamate-induced cytotoxicity was determined

IC ICM A61K031-00

ICS A61K031-165; A61K031-55; A61K031-645

CC 1-11 (Pharmacology)

IT Capsaicin receptors

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(antagonists or partial agonists of vanilloid receptor complexes for treating neurodegenerative diseases)

IT Nerve, disease

(neuropathy, peripheral, inhibition of; antagonists or partial agonists of vanilloid receptor complexes for treating neurodegenerative diseases)

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L168 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:811082 HCAPLUS Full-text

DOCUMENT NUMBER: 130:218085

TITLE: Anandamide transport inhibition by the vanilloid agonist olvanil

AUTHOR(S): Beltramo, Massimiliano; Piomelli, Daniele

CORPORATE SOURCE: The Neurosciences Institute, San Diego, CA, 92121, USA

SOURCE: European Journal of Pharmacology (1999),  
364(1), 75-78

CODEN: EJPHAZ; ISSN: 0014-2999

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The structural similarities between the anandamide transport inhibitor N-(4-hydroxyphenyl)-arachidonamide (AM404) and the synthetic vanilloid agonist olvanil [(N-vanillyl)-9-oleamide], prompted us to investigate the possibility that olvanil may interfere with anandamide transport. The intracellular accumulation of [3H]anandamide by human astrocytoma cells was prevented by olvanil with a  $K_i$  value of  $14.1 \pm 7.1$   $\mu$ M. By contrast, capsaicin [(8-methyl-N-vanillyl)-6-noneamide], a plant-derived vanilloid agonist, and capsazepine (N-[2-(4-chlorophenyl)ethyl]-1,3,4,5-tetrahydro-7,8-dihydroxy-2H-2-benzazepine-2-carbothioamide), a vanilloid antagonist, had no such effect ( $K_i > 100$   $\mu$ M). These results indicate that, although less potent than AM404 ( $K_i$   $2.1 \pm 0.2$   $\mu$ M), olvanil may reduce anandamide clearance at concns. similar to those needed for vanilloid receptor activation.

CC 1-11 (Pharmacology)

ST anandamide transport olvanil analgesic vanilloid receptor

IT Analgesics

Astrocyte

(anandamide transport inhibition by vanilloid agonist olvanil)

L168 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:304897 HCAPLUS Full-text

DOCUMENT NUMBER: 126:338728

TITLE: The selective capsaicin antagonist capsazepine abolishes the antinociceptive action of eugenol and guaiacol

AUTHOR(S): Ohkubo, T.; Shibata, M.

CORPORATE SOURCE: Dept. Pharmacology, Fukuoka Dental College, Fukuoka, 814-01, Japan

SOURCE: Journal of Dental Research (1997), 76(4), 848-851

CODEN: JDREAF; ISSN: 0022-0345

PUBLISHER: International Association for Dental Research

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The dental phenolic medicaments, eugenol and guaiacol, are partly similar in chemical structure to capsaicin, the pungent constituent of chili peppers, which selectively activates sensory neurons via a specific receptor. We have previously demonstrated that these phenolic compds. show capsaicin-like action. In the present study, an attempt was made to investigate the possibility that these compds. interact with the same cellular site as capsaicin, by using capsazepine, a selective and competitive antagonist of capsaicin. Intrathecal (i.t.) treatment with eugenol (12.5 to 50 µg), guaiacol (25 to 150 µg), or capsaicin (1 to 4 µg) for 24 h dose-dependently inhibited the formalin-induced nociceptive response. Capsazepine (5, 10 µg, i.t.) shifted these dose-response curves in parallel to the right. Similarly, capsazepine abolished antinociceptive effects of eugenol (50 µg), guaiacol (150 µg) in the acetic acid writhing test. These results suggest that eugenol and guaiacol may exert their antinociceptive effects via the capsaicin receptor located on sensory terminals in the spinal cord.

CC 1-11 (Pharmacology)

IT Analgesics

Spinal cord

(the selective capsaicin antagonist capsazepine abolishes the antinociceptive action of eugenol and guaiacol)

IT Capsaicin receptors

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(the selective capsaicin antagonist capsazepine abolishes the antinociceptive action of eugenol and guaiacol)

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

FILE 'HOME' ENTERED AT 15:54:39 ON 30 JAN 2008



NSPEC IS R AT 4  
 NSPEC IS RC AT 5  
 CONNECT IS E1 RC AT 22  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 38

STEREO ATTRIBUTES: NONE  
 L93 8317 SEA FILE=REGISTRY SUB=L85 SSS FUL (L50 NOT (L87 OR L88 OR L89  
 OR L90))

100.0% PROCESSED 111701 ITERATIONS  
 SEARCH TIME: 00.00.13

8317 ANSWERS

(FILE 'LREGISTRY' ENTERED AT 09:57:02 ON 30 JAN 2008)  
 DEL HIS Y

FILE 'ZCAPLUS' ENTERED AT 11:43:46 ON 30 JAN 2008  
 E PAIN+ALL/CT

FILE 'ZCAPLUS' ENTERED AT 11:44:02 ON 30 JAN 2008  
 E US2004-799286/APPS

L1 1 SEA ABB=ON US2004-799286/AP  
 D SCAN  
 SEL RN

FILE 'REGISTRY' ENTERED AT 11:44:56 ON 30 JAN 2008

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L36 FILE 'REGISTRY' ENTERED AT 12:21:18 ON 30 JAN 2008  
 TRA L35 1- RN : 50700 TERMS (TERM LIMIT EXCEEDED)

L37 FILE 'REGISTRY, REGISTRY' ENTERED AT 12:21:18 ON 30 JAN 2008  
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FILE 'STNGUIDE' ENTERED AT 12:26:54 ON 30 JAN 2008

L38 FILE 'REGISTRY' ENTERED AT 12:32:35 ON 30 JAN 2008  
 L39 STR L3  
 50 SEA SSS SAM L38

FILE 'STNGUIDE' ENTERED AT 12:39:04 ON 30 JAN 2008

L40 FILE 'REGISTRY' ENTERED AT 12:46:21 ON 30 JAN 2008  
 L41 STR L39  
 L42 STR L40  
 L43 SCREEN 1839 AND 1993  
 L44 SCREEN 219 OR 218  
 L45 8 SEA SSS SAM (L38 NOT ((L40 OR L41))) AND L42 AND L43  
 L46 STR L38  
 L47 STR L45  
 L48 STR L46  
 7 SEA SSS SAM (L38 NOT ((L40 OR L41 OR L46 OR L47))) AND L42 AND  
 L43  
 D SCAN  
 L49 STR L38  
 L50 STR L49  
 L51 6 SEA SSS SAM (L50 NOT ((L40 OR L41 OR L46 OR L47))) AND L42 AND  
 L43

FILE 'STNGUIDE' ENTERED AT 14:35:51 ON 30 JAN 2008

L52 FILE 'REGISTRY' ENTERED AT 14:43:25 ON 30 JAN 2008  
 L53 SCREEN 392 OR 391  
 L54 SCREEN 2043 OR 2049  
 10 SEA SSS SAM (L50 NOT ((L40 OR L41 OR L46 OR L47))) AND L42 AND  
 L52 NOT L53  
 D SCAN

FILE 'STNGUIDE' ENTERED AT 14:45:51 ON 30 JAN 2008

FILE 'REGISTRY' ENTERED AT 14:47:01 ON 30 JAN 2008  
 E RSD/FA  
 E PS/FS  
 E NS/FS

FILE 'STNGUIDE' ENTERED AT 14:49:32 ON 30 JAN 2008

FILE 'REGISTRY' ENTERED AT 14:49:54 ON 30 JAN 2008

L93 8317 SEA SUB=L85 SSS FUL (L50 NOT (L87 OR L88 OR L89 OR L90))  
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FILE 'HCAPLUS' ENTERED AT 15:14:00 ON 30 JAN 2008

L94 1407 SEA ABB=ON L93  
 L95 1 SEA ABB=ON L94 AND (L5 OR L6 OR L7 OR L8 OR L9 OR L10 OR L11)

D SCAN TI  
 D SCAN TI L5

L96 2 SEA ABB=ON (L95 OR L5)  
 L97 136 SEA ABB=ON (L12 OR L13 OR L14 OR L15 OR L16 OR L17 OR L18 OR  
 L19 OR L20 OR L21 OR L22 OR L23 OR L24 OR L25 OR L26 OR L27 OR  
 L28 OR L29 OR L30 OR L31 OR L32 OR L33 OR L34) AND L94

L98 9 SEA ABB=ON L32 AND L94  
 L99 16 SEA ABB=ON L94 AND L12  
 L100 3 SEA ABB=ON L94 AND L13  
 L101 4 SEA ABB=ON L94 AND L14  
 L102 0 SEA ABB=ON L94 AND L15  
 L103 0 SEA ABB=ON L94 AND L16  
 L104 0 SEA ABB=ON L94 AND L17  
 L105 29 SEA ABB=ON L94 AND L18  
 L106 0 SEA ABB=ON L94 AND L19  
 L107 0 SEA ABB=ON L94 AND L20  
 L108 0 SEA ABB=ON L94 AND L21  
 L109 81 SEA ABB=ON L94 AND L22  
 L110 1 SEA ABB=ON L94 AND L23  
 L111 0 SEA ABB=ON L94 AND L24  
 L112 0 SEA ABB=ON L94 AND L25  
 L113 0 SEA ABB=ON L94 AND L26  
 L114 16 SEA ABB=ON L94 AND L27  
 L115 0 SEA ABB=ON L94 AND L28  
 L116 4 SEA ABB=ON L94 AND L29  
 L117 0 SEA ABB=ON L94 AND L30  
 L118 9 SEA ABB=ON L94 AND L31  
 L119 1 SEA ABB=ON L94 AND L33  
 L120 46 SEA ABB=ON L94 AND L34  
 L121 24 SEA ABB=ON L94 AND (L13 OR L14 OR L15 OR L16 OR L17 OR L19 OR  
 L20 OR L21 OR L23 OR L24 OR L25 OR L26 OR L28 OR L29 OR L30 OR  
 L31 OR L32 OR L33)

L122 573 SEA ABB=ON L94(L) (THU OR BAC OR PAC OR PKT OR DMA)/RL  
 L123 37 SEA ABB=ON L122 AND (L12 OR L18 OR L27)  
 L124 12 SEA ABB=ON L122 AND L12  
 L125 27 SEA ABB=ON L122 AND L18  
 L126 73 SEA ABB=ON L122 AND L22  
 L127 11 SEA ABB=ON L122 AND L27  
 L128 33 SEA ABB=ON L122 AND L34  
 L129 4634 SEA ABB=ON (L12 AND (L18 OR L22 OR L27 OR L34))  
 L130 912 SEA ABB=ON L94 AND (PY<2001 OR AY<2001 OR PRY<2001)  
 L131 268 SEA ABB=ON L130 AND L122  
 L132 27 SEA ABB=ON L131 AND (L12 OR L18 OR L22 OR L27 OR L34)  
 L133 0 SEA ABB=ON L98 AND L130  
 L134 2 SEA ABB=ON L121 AND L130  
 L135 40 SEA ABB=ON L130 AND (L12 OR L18 OR L22 OR L27 OR L34)  
 L136 9 SEA ABB=ON L94(L) (L12 OR L13 OR L14 OR L15 OR L16 OR L17 OR  
 L19 OR L20 OR L21 OR L22 OR L23 OR L24 OR L25 OR L26 OR L27 OR  
 L28 OR L29 OR L30 OR L31 OR L33 OR L34)

L137 2 SEA ABB=ON L94(L) (L12 OR L13 OR L14 OR L15 OR L16 OR L17 OR  
 L19 OR L20 OR L21 OR L22 OR L23 OR L24 OR L25 OR L26 OR L27 OR  
 L28 OR L29 OR L30 OR L31 OR L33 OR L34) AND L130  
 D SCAN

L166 18828 SEA ABB=ON (L160 OR L151 OR L158) NOT (L96 OR L163 OR L164 OR  
L165)  
D QUE NOS L157  
D QUE NOS L160  
D QUE NOS L157  
D QUE NOS L158  
L167 21 SEA ABB=ON (L160 OR L157 OR L158) NOT (L96 OR L163 OR L164 OR  
L165)  
D IBIB ABS HITIND HITSTR L167 1-21

FILE 'HCAPLUS' ENTERED AT 15:54:01 ON 30 JAN 2008

D QUE L162

L168 9 SEA ABB=ON L162 NOT (L96 OR L163 OR L164 OR L165 OR L167)  
D IBIB ABS HITIND 1-9

FILE 'HOME' ENTERED AT 15:54:39 ON 30 JAN 2008

D STAT QUE L93

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